



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 01:56 PM BST

PDB ID : 5NFF
Title : Crystal structure of GP1 receptor binding domain from Morogoro virus
Authors : Israeli, H.; Cohen-Dvashi, H.; Shulman, A.; Shimon, A.; Diskin, R.
Deposited on : 2017-03-14
Resolution : 2.62 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.13.1
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) : 2.13.1

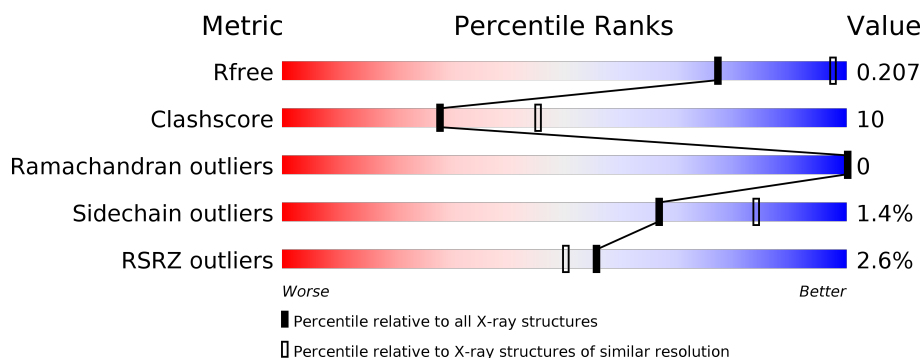
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	171	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>9%</div> </div> </div>
1	B	171	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>9%</div> </div> </div>
1	C	171	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>• 9%</div> </div> </div>
1	D	171	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>22%</div> <div>• 9%</div> </div> </div>
1	E	171	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>9%</div> </div> </div>
1	F	171	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• 9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	171	
1	H	171	
1	I	171	
1	J	171	
1	K	171	
1	L	171	
1	M	171	
1	N	171	
1	O	171	
1	P	171	
2	Q	2	
2	R	2	
3	S	4	
4	T	5	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 20391 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 Glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	156	Total	C	N	O	S	0	0	0
			1246	779	215	241	11			
1	A	156	Total	C	N	O	S	0	0	0
			1246	779	215	241	11			
1	C	156	Total	C	N	O	S	0	0	0
			1246	779	215	241	11			
1	D	156	Total	C	N	O	S	0	0	0
			1246	779	215	241	11			
1	E	156	Total	C	N	O	S	0	0	0
			1246	779	215	241	11			
1	F	156	Total	C	N	O	S	0	0	0
			1246	779	215	241	11			
1	G	156	Total	C	N	O	S	0	0	0
			1246	779	215	241	11			
1	H	156	Total	C	N	O	S	0	0	0
			1246	779	215	241	11			
1	I	156	Total	C	N	O	S	0	0	0
			1246	779	215	241	11			
1	J	156	Total	C	N	O	S	0	0	0
			1246	779	215	241	11			
1	K	156	Total	C	N	O	S	0	0	0
			1246	779	215	241	11			
1	L	156	Total	C	N	O	S	0	0	0
			1246	779	215	241	11			
1	M	156	Total	C	N	O	S	0	0	0
			1246	779	215	241	11			
1	N	156	Total	C	N	O	S	0	0	0
			1246	779	215	241	11			
1	O	156	Total	C	N	O	S	0	0	0
			1246	779	215	241	11			
1	P	156	Total	C	N	O	S	0	0	0
			1246	779	215	241	11			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	65	SER	-	expression tag	UNP C6ZK00
B	66	HIS	-	expression tag	UNP C6ZK00
B	67	HIS	-	expression tag	UNP C6ZK00
B	68	HIS	-	expression tag	UNP C6ZK00
B	69	HIS	-	expression tag	UNP C6ZK00
B	70	HIS	-	expression tag	UNP C6ZK00
B	71	HIS	-	expression tag	UNP C6ZK00
B	72	GLY	-	expression tag	UNP C6ZK00
B	73	GLY	-	expression tag	UNP C6ZK00
A	65	SER	-	expression tag	UNP C6ZK00
A	66	HIS	-	expression tag	UNP C6ZK00
A	67	HIS	-	expression tag	UNP C6ZK00
A	68	HIS	-	expression tag	UNP C6ZK00
A	69	HIS	-	expression tag	UNP C6ZK00
A	70	HIS	-	expression tag	UNP C6ZK00
A	71	HIS	-	expression tag	UNP C6ZK00
A	72	GLY	-	expression tag	UNP C6ZK00
A	73	GLY	-	expression tag	UNP C6ZK00
C	65	SER	-	expression tag	UNP C6ZK00
C	66	HIS	-	expression tag	UNP C6ZK00
C	67	HIS	-	expression tag	UNP C6ZK00
C	68	HIS	-	expression tag	UNP C6ZK00
C	69	HIS	-	expression tag	UNP C6ZK00
C	70	HIS	-	expression tag	UNP C6ZK00
C	71	HIS	-	expression tag	UNP C6ZK00
C	72	GLY	-	expression tag	UNP C6ZK00
C	73	GLY	-	expression tag	UNP C6ZK00
D	65	SER	-	expression tag	UNP C6ZK00
D	66	HIS	-	expression tag	UNP C6ZK00
D	67	HIS	-	expression tag	UNP C6ZK00
D	68	HIS	-	expression tag	UNP C6ZK00
D	69	HIS	-	expression tag	UNP C6ZK00
D	70	HIS	-	expression tag	UNP C6ZK00
D	71	HIS	-	expression tag	UNP C6ZK00
D	72	GLY	-	expression tag	UNP C6ZK00
D	73	GLY	-	expression tag	UNP C6ZK00
E	65	SER	-	expression tag	UNP C6ZK00
E	66	HIS	-	expression tag	UNP C6ZK00
E	67	HIS	-	expression tag	UNP C6ZK00
E	68	HIS	-	expression tag	UNP C6ZK00
E	69	HIS	-	expression tag	UNP C6ZK00
E	70	HIS	-	expression tag	UNP C6ZK00

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Chain	Residue	Modelled	Actual	Comment	Reference
E	71	HIS	-	expression tag	UNP C6ZK00
E	72	GLY	-	expression tag	UNP C6ZK00
E	73	GLY	-	expression tag	UNP C6ZK00
F	65	SER	-	expression tag	UNP C6ZK00
F	66	HIS	-	expression tag	UNP C6ZK00
F	67	HIS	-	expression tag	UNP C6ZK00
F	68	HIS	-	expression tag	UNP C6ZK00
F	69	HIS	-	expression tag	UNP C6ZK00
F	70	HIS	-	expression tag	UNP C6ZK00
F	71	HIS	-	expression tag	UNP C6ZK00
F	72	GLY	-	expression tag	UNP C6ZK00
F	73	GLY	-	expression tag	UNP C6ZK00
G	65	SER	-	expression tag	UNP C6ZK00
G	66	HIS	-	expression tag	UNP C6ZK00
G	67	HIS	-	expression tag	UNP C6ZK00
G	68	HIS	-	expression tag	UNP C6ZK00
G	69	HIS	-	expression tag	UNP C6ZK00
G	70	HIS	-	expression tag	UNP C6ZK00
G	71	HIS	-	expression tag	UNP C6ZK00
G	72	GLY	-	expression tag	UNP C6ZK00
G	73	GLY	-	expression tag	UNP C6ZK00
H	65	SER	-	expression tag	UNP C6ZK00
H	66	HIS	-	expression tag	UNP C6ZK00
H	67	HIS	-	expression tag	UNP C6ZK00
H	68	HIS	-	expression tag	UNP C6ZK00
H	69	HIS	-	expression tag	UNP C6ZK00
H	70	HIS	-	expression tag	UNP C6ZK00
H	71	HIS	-	expression tag	UNP C6ZK00
H	72	GLY	-	expression tag	UNP C6ZK00
H	73	GLY	-	expression tag	UNP C6ZK00
I	65	SER	-	expression tag	UNP C6ZK00
I	66	HIS	-	expression tag	UNP C6ZK00
I	67	HIS	-	expression tag	UNP C6ZK00
I	68	HIS	-	expression tag	UNP C6ZK00
I	69	HIS	-	expression tag	UNP C6ZK00
I	70	HIS	-	expression tag	UNP C6ZK00
I	71	HIS	-	expression tag	UNP C6ZK00
I	72	GLY	-	expression tag	UNP C6ZK00
I	73	GLY	-	expression tag	UNP C6ZK00
J	65	SER	-	expression tag	UNP C6ZK00
J	66	HIS	-	expression tag	UNP C6ZK00
J	67	HIS	-	expression tag	UNP C6ZK00

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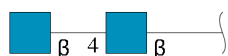
Chain	Residue	Modelled	Actual	Comment	Reference
J	68	HIS	-	expression tag	UNP C6ZK00
J	69	HIS	-	expression tag	UNP C6ZK00
J	70	HIS	-	expression tag	UNP C6ZK00
J	71	HIS	-	expression tag	UNP C6ZK00
J	72	GLY	-	expression tag	UNP C6ZK00
J	73	GLY	-	expression tag	UNP C6ZK00
K	65	SER	-	expression tag	UNP C6ZK00
K	66	HIS	-	expression tag	UNP C6ZK00
K	67	HIS	-	expression tag	UNP C6ZK00
K	68	HIS	-	expression tag	UNP C6ZK00
K	69	HIS	-	expression tag	UNP C6ZK00
K	70	HIS	-	expression tag	UNP C6ZK00
K	71	HIS	-	expression tag	UNP C6ZK00
K	72	GLY	-	expression tag	UNP C6ZK00
K	73	GLY	-	expression tag	UNP C6ZK00
L	65	SER	-	expression tag	UNP C6ZK00
L	66	HIS	-	expression tag	UNP C6ZK00
L	67	HIS	-	expression tag	UNP C6ZK00
L	68	HIS	-	expression tag	UNP C6ZK00
L	69	HIS	-	expression tag	UNP C6ZK00
L	70	HIS	-	expression tag	UNP C6ZK00
L	71	HIS	-	expression tag	UNP C6ZK00
L	72	GLY	-	expression tag	UNP C6ZK00
L	73	GLY	-	expression tag	UNP C6ZK00
M	65	SER	-	expression tag	UNP C6ZK00
M	66	HIS	-	expression tag	UNP C6ZK00
M	67	HIS	-	expression tag	UNP C6ZK00
M	68	HIS	-	expression tag	UNP C6ZK00
M	69	HIS	-	expression tag	UNP C6ZK00
M	70	HIS	-	expression tag	UNP C6ZK00
M	71	HIS	-	expression tag	UNP C6ZK00
M	72	GLY	-	expression tag	UNP C6ZK00
M	73	GLY	-	expression tag	UNP C6ZK00
N	65	SER	-	expression tag	UNP C6ZK00
N	66	HIS	-	expression tag	UNP C6ZK00
N	67	HIS	-	expression tag	UNP C6ZK00
N	68	HIS	-	expression tag	UNP C6ZK00
N	69	HIS	-	expression tag	UNP C6ZK00
N	70	HIS	-	expression tag	UNP C6ZK00
N	71	HIS	-	expression tag	UNP C6ZK00
N	72	GLY	-	expression tag	UNP C6ZK00
N	73	GLY	-	expression tag	UNP C6ZK00

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Chain	Residue	Modelled	Actual	Comment	Reference
O	65	SER	-	expression tag	UNP C6ZK00
O	66	HIS	-	expression tag	UNP C6ZK00
O	67	HIS	-	expression tag	UNP C6ZK00
O	68	HIS	-	expression tag	UNP C6ZK00
O	69	HIS	-	expression tag	UNP C6ZK00
O	70	HIS	-	expression tag	UNP C6ZK00
O	71	HIS	-	expression tag	UNP C6ZK00
O	72	GLY	-	expression tag	UNP C6ZK00
O	73	GLY	-	expression tag	UNP C6ZK00
P	65	SER	-	expression tag	UNP C6ZK00
P	66	HIS	-	expression tag	UNP C6ZK00
P	67	HIS	-	expression tag	UNP C6ZK00
P	68	HIS	-	expression tag	UNP C6ZK00
P	69	HIS	-	expression tag	UNP C6ZK00
P	70	HIS	-	expression tag	UNP C6ZK00
P	71	HIS	-	expression tag	UNP C6ZK00
P	72	GLY	-	expression tag	UNP C6ZK00
P	73	GLY	-	expression tag	UNP C6ZK00

- Molecule 2 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
2	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



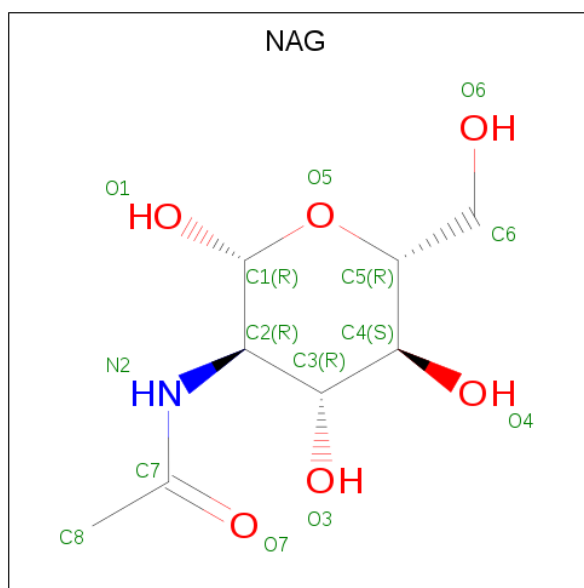
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	S	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	T	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



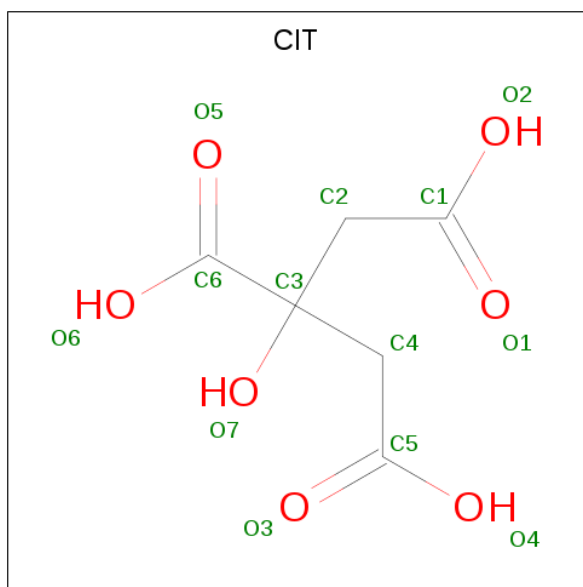
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).

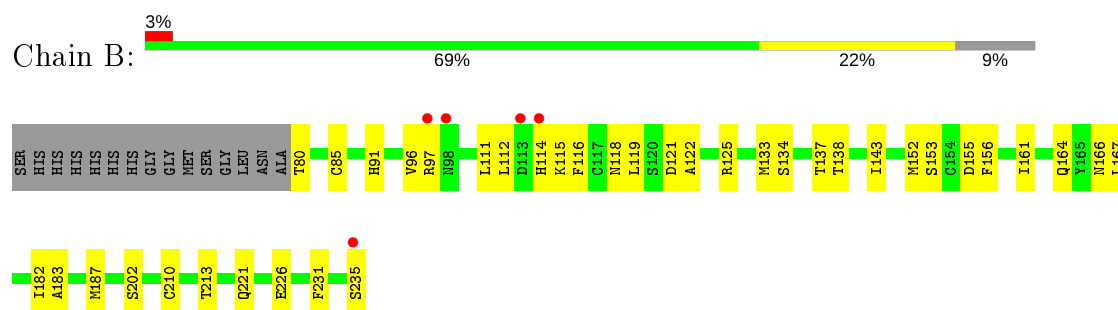


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 13	C 6	O 7	0	0
6	C	1	Total 13	C 6	O 7	0	0
6	C	1	Total 13	C 6	O 7	0	0
6	E	1	Total 13	C 6	O 7	0	0
6	F	1	Total 13	C 6	O 7	0	0
6	I	1	Total 13	C 6	O 7	0	0

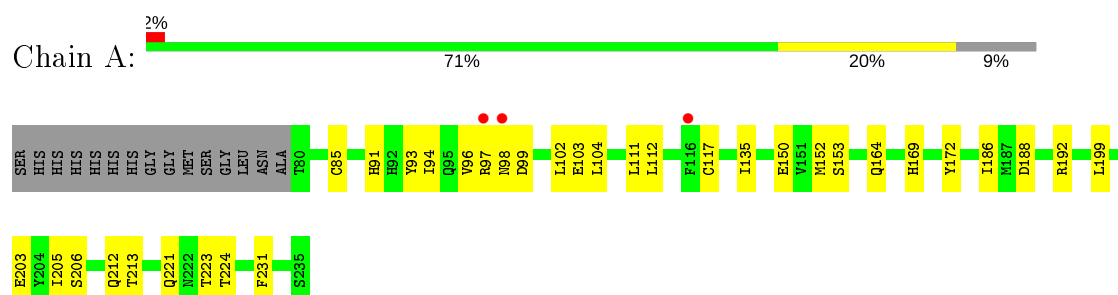
3 Residue-property plots [i](#)

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.

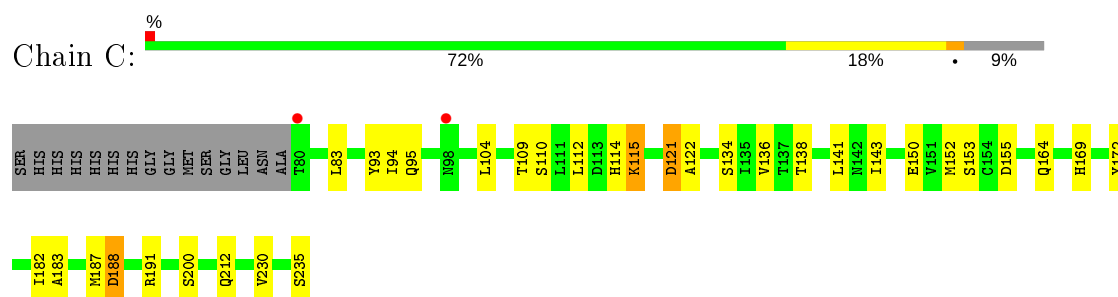
- Molecule 1: Glycoprotein



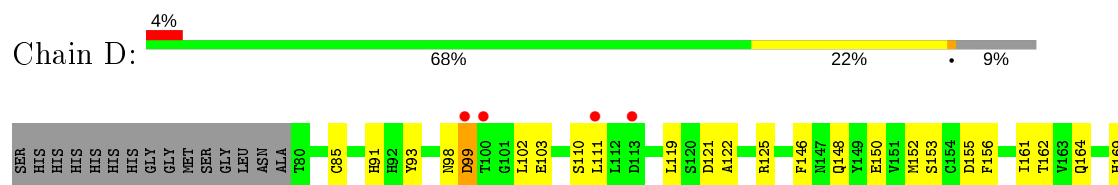
- Molecule 1: Glycoprotein



- Molecule 1: Glycoprotein



- Molecule 1: Glycoprotein

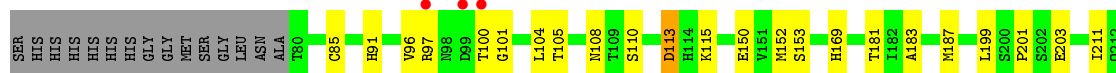
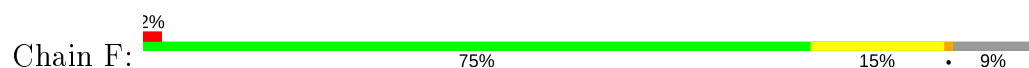




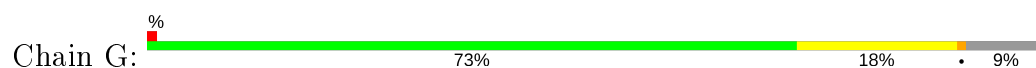
• Molecule 1: Glycoprotein



• Molecule 1: Glycoprotein



• Molecule 1: Glycoprotein

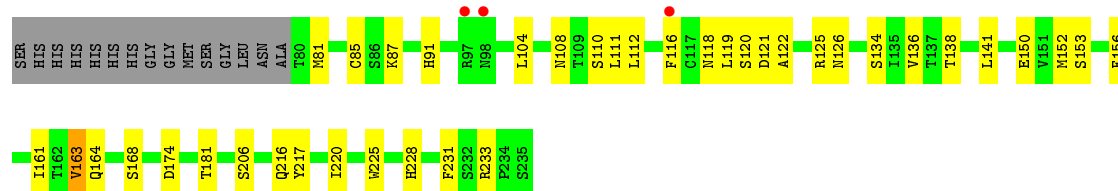


• Molecule 1: Glycoprotein

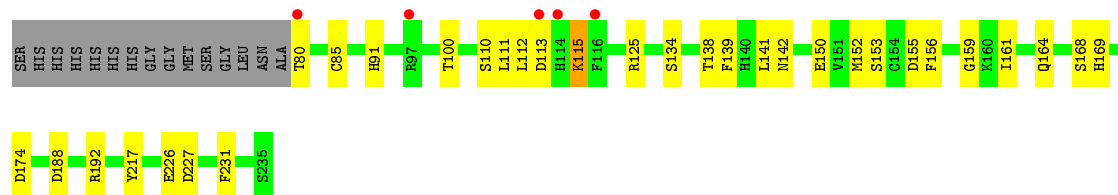


• Molecule 1: Glycoprotein

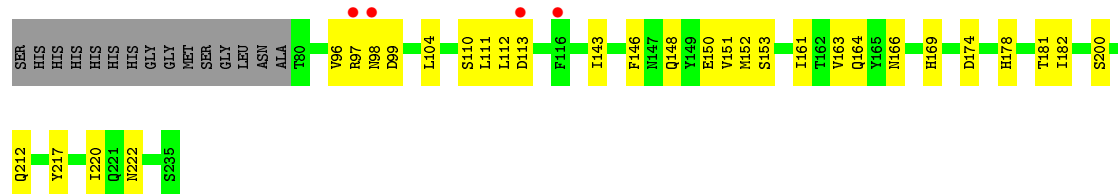
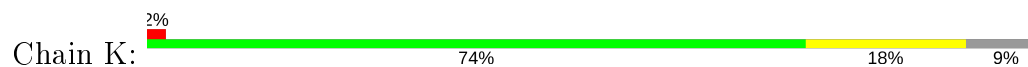




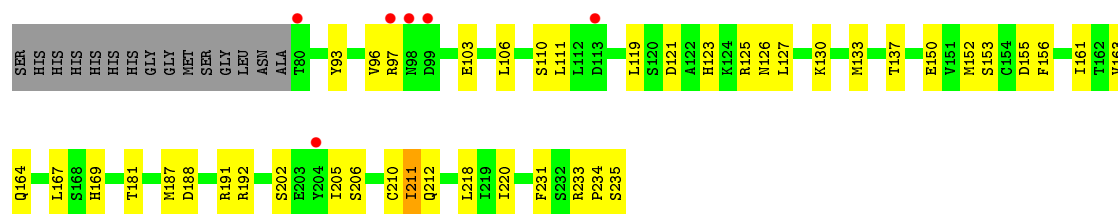
• Molecule 1: Glycoprotein



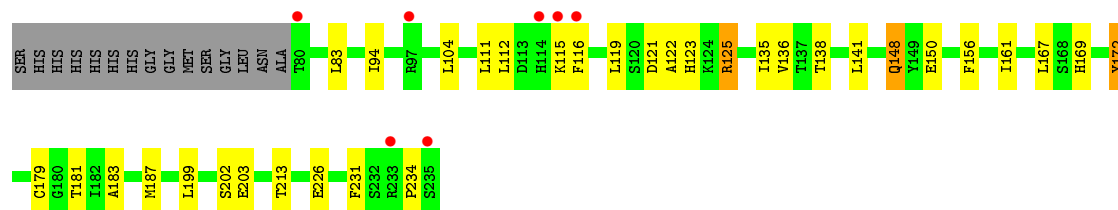
• Molecule 1: Glycoprotein



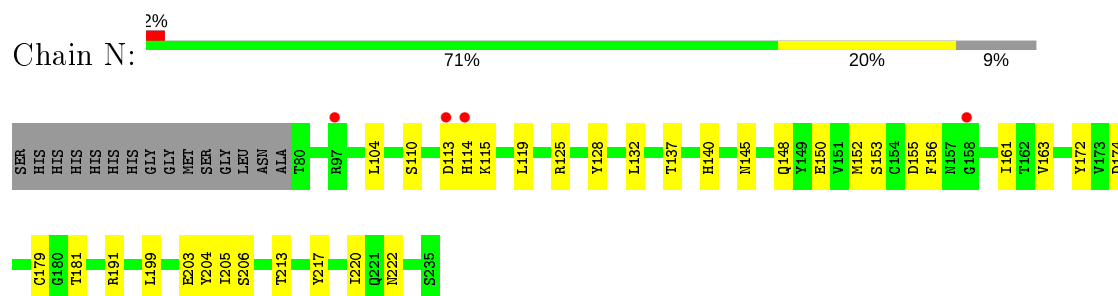
• Molecule 1: Glycoprotein



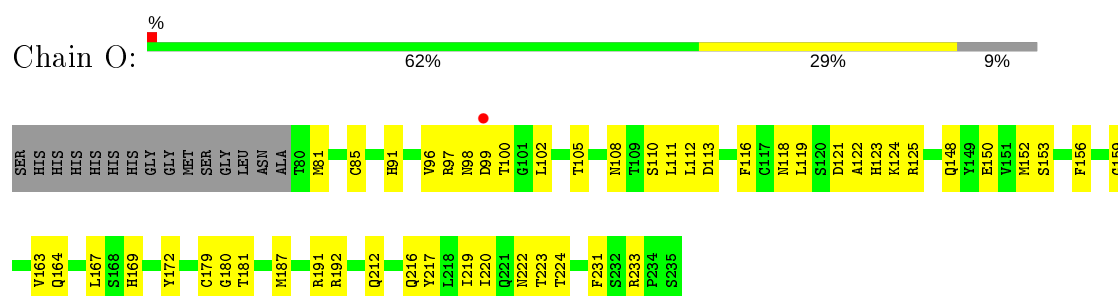
• Molecule 1: Glycoprotein



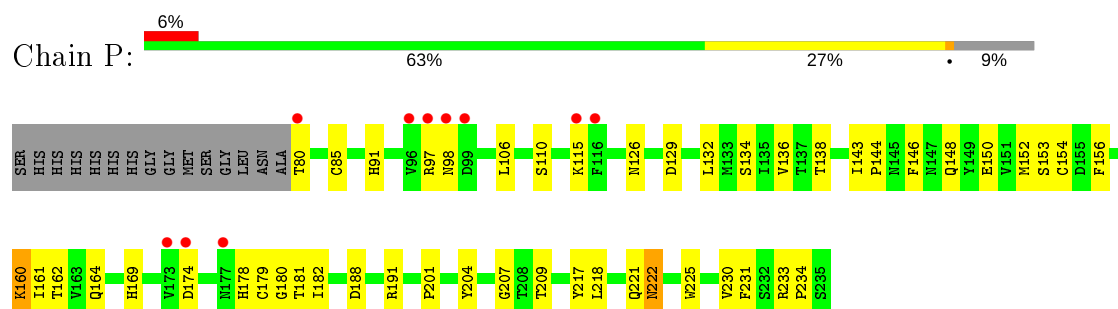
- Molecule 1: Glycoprotein



- Molecule 1: Glycoprotein



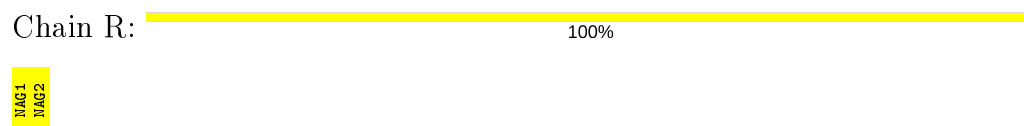
- Molecule 1: Glycoprotein




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



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



- Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  75% 25%

HA01
HA02
MAN3
MAN4

- Molecule 4: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  20% 80%

HA01
HA02
MAN3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	127.77Å 127.77Å 251.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.19 – 2.62 46.19 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.19-2.62) 99.6 (46.19-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.75 (at 2.61Å)	Xtriage
Refinement program	PHENIX dev_2236	Depositor
R, R_{free}	0.174 , 0.207 0.174 , 0.207	Depositor DCC
R_{free} test set	6982 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l 0.048 for h,-h-k,-l 0.012 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20391	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: CIT, NAG, MAN

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	0.46	1/1276 (0.1%)	0.67	0/1735
1	B	0.52	0/1276	0.69	0/1735
1	C	0.50	0/1276	0.69	2/1735 (0.1%)
1	D	0.42	0/1276	0.66	1/1735 (0.1%)
1	E	0.46	0/1276	0.69	0/1735
1	F	0.48	1/1276 (0.1%)	0.65	0/1735
1	G	0.47	0/1276	0.68	1/1735 (0.1%)
1	H	0.38	0/1276	0.65	0/1735
1	I	0.51	0/1276	0.66	0/1735
1	J	0.45	0/1276	0.70	1/1735 (0.1%)
1	K	0.60	0/1276	0.69	0/1735
1	L	0.38	0/1276	0.63	0/1735
1	M	0.50	0/1276	0.67	1/1735 (0.1%)
1	N	0.36	0/1276	0.57	0/1735
1	O	0.47	0/1276	0.67	0/1735
1	P	0.43	0/1276	0.68	1/1735 (0.1%)
All	All	0.47	2/20416 (0.0%)	0.67	7/27760 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	P	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	108	ASN	CB-CG	6.65	1.66	1.51
1	A	117	CYS	CB-SG	5.11	1.91	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	80	THR	N-CA-C	-7.04	91.98	111.00
1	P	160	LYS	CD-CE-NZ	-6.17	97.50	111.70
1	M	125	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	121	ASP	CB-CG-OD2	5.68	123.41	118.30
1	G	113	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	99	ASP	CB-CG-OD1	5.32	123.08	118.30
1	C	188	ASP	CB-CG-OD2	5.09	122.88	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	115	LYS	Peptide
1	P	115	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1246	0	1174	23	0
1	B	1246	0	1173	26	0
1	C	1246	0	1175	20	0
1	D	1246	0	1175	30	0
1	E	1246	0	1174	20	0
1	F	1246	0	1175	16	0
1	G	1246	0	1174	23	0
1	H	1246	0	1174	25	0
1	I	1246	0	1175	27	0
1	J	1246	0	1175	23	0
1	K	1246	0	1175	19	0
1	L	1246	0	1175	29	0
1	M	1246	0	1176	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1246	0	1176	24	0
1	O	1246	0	1175	39	0
1	P	1246	0	1176	37	0
2	Q	28	0	25	2	0
2	R	28	0	25	0	0
3	S	50	0	43	2	0
4	T	61	0	52	3	0
5	A	28	0	26	1	0
5	B	28	0	26	0	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
5	E	28	0	26	1	0
5	G	28	0	26	1	0
5	H	14	0	13	0	0
5	I	14	0	13	0	0
5	J	14	0	13	3	0
5	K	14	0	13	0	0
5	L	14	0	13	0	0
6	B	13	0	5	0	0
6	C	26	0	10	2	0
6	E	13	0	5	0	0
6	F	13	0	5	1	0
6	I	13	0	5	0	0
All	All	20391	0	19167	391	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 (391) 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:I:81:MET:HE1	1:I:233:ARG:HG2	1.40	1.03
1:I:81:MET:HG2	1:I:231:PHE:O	1.66	0.95
1:I:81:MET:CE	1:I:233:ARG:HG2	1.98	0.93
1:C:188:ASP:OD1	1:C:191:ARG:NH1	2.03	0.91
1:M:150:GLU:OE2	1:M:169:HIS:NE2	2.10	0.85
1:N:148:GLN:HE22	1:N:179:CYS:H	1.26	0.81
1:A:94:ILE:HD11	1:A:102:LEU:HD12	1.65	0.79
1:P:97:ARG:HG3	1:P:98:ASN:H	1.48	0.79
1:E:96:VAL:HG21	5:E:301:NAG:H83	1.64	0.77
1:K:163:VAL:HG12	1:K:220:ILE:HB	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:184:ASN:HD21	1:G:211:ILE:H	1.31	0.75
1:J:100:THR:HG21	5:J:301:NAG:HN2	1.51	0.75
1:I:163:VAL:HG13	1:I:220:ILE:HB	1.68	0.75
1:O:98:ASN:OD1	1:O:99:ASP:N	2.18	0.75
1:D:111:LEU:H	1:D:164:GLN:HE22	1.33	0.74
1:M:150:GLU:HG2	1:M:181:THR:HG21	1.69	0.74
1:J:113:ASP:O	1:J:115:LYS:NZ	2.21	0.73
1:A:188:ASP:OD2	1:A:192:ARG:NH1	2.20	0.73
1:O:96:VAL:HG23	1:O:97:ARG:HG2	1.70	0.73
1:D:203:GLU:OE1	1:G:200:SER:HB2	1.88	0.73
1:G:96:VAL:HG21	5:G:302:NAG:H83	1.69	0.73
1:B:134:SER:O	1:B:138:THR:HG23	1.88	0.73
2:Q:1:NAG:H61	2:Q:2:NAG:O5	1.89	0.73
1:J:188:ASP:O	1:J:192:ARG:HG3	1.89	0.73
1:E:121:ASP:OD1	1:E:123:HIS:HB3	1.88	0.72
1:J:152:MET:HG2	1:J:153:SER:N	2.01	0.72
1:C:150:GLU:N	6:C:303:CIT:O3	2.22	0.71
1:D:150:GLU:OE2	1:D:169:HIS:HE1	1.73	0.70
1:B:152:MET:HG2	1:B:153:SER:N	2.06	0.70
1:B:226:GLU:N	1:B:226:GLU:OE1	2.25	0.69
1:K:143:ILE:HG13	1:K:182:ILE:HD13	1.75	0.69
1:N:119:LEU:HB3	1:N:125:ARG:HG2	1.74	0.69
1:H:134:SER:O	1:H:138:THR:OG1	2.11	0.68
1:A:152:MET:HG2	1:A:153:SER:N	2.09	0.68
1:D:111:LEU:H	1:D:164:GLN:NE2	1.91	0.68
1:N:128:TYR:OH	1:N:152:MET:SD	2.51	0.68
1:H:96:VAL:HG23	1:H:97:ARG:HG2	1.75	0.68
1:A:150:GLU:OE2	1:A:169:HIS:NE2	2.24	0.67
1:F:113:ASP:N	1:F:113:ASP:OD1	2.26	0.67
1:P:143:ILE:HG13	1:P:182:ILE:HG12	1.75	0.67
1:O:148:GLN:HE22	1:O:179:CYS:H	1.43	0.67
1:O:111:LEU:H	1:O:164:GLN:NE2	1.93	0.66
1:B:187:MET:HE1	1:B:213:THR:HG21	1.76	0.66
1:I:104:LEU:HD22	1:I:220:ILE:HG12	1.78	0.66
1:L:96:VAL:HG23	1:L:97:ARG:HG2	1.76	0.66
1:C:152:MET:HG2	1:C:153:SER:N	2.11	0.66
1:A:96:VAL:HG23	1:A:97:ARG:HG2	1.78	0.66
1:C:114:HIS:C	1:C:115:LYS:HE2	2.17	0.65
1:L:126:ASN:HD21	1:L:130:LYS:NZ	1.94	0.65
1:L:150:GLU:HG2	1:L:181:THR:HG21	1.78	0.65
1:L:150:GLU:OE1	1:L:169:HIS:NE2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:124:LYS:HB2	1:O:156:PHE:CZ	2.32	0.65
1:I:85:CYS:HA	1:I:91:HIS:CD2	2.32	0.65
1:I:206:SER:OG	1:L:126:ASN:ND2	2.29	0.65
1:P:160:LYS:NZ	1:P:222:ASN:O	2.31	0.64
1:P:148:GLN:HE22	1:P:179:CYS:H	1.46	0.64
1:D:203:GLU:OE2	1:D:205:ILE:HD11	1.98	0.64
1:M:226:GLU:HA	1:P:230:VAL:HG21	1.80	0.64
1:K:112:LEU:H	1:K:164:GLN:HE22	1.46	0.63
1:P:97:ARG:HG3	1:P:98:ASN:N	2.12	0.63
1:O:121:ASP:OD1	1:O:122:ALA:N	2.31	0.63
1:D:119:LEU:HD22	1:D:125:ARG:HA	1.80	0.63
1:B:114:HIS:HB2	1:B:116:PHE:CD1	2.34	0.63
1:E:169:HIS:O	1:E:212:GLN:HG2	1.99	0.62
1:O:96:VAL:HG23	1:O:97:ARG:N	2.14	0.62
6:C:303:CIT:O4	6:C:303:CIT:O7	2.15	0.62
1:G:104:LEU:HD22	1:G:220:ILE:HG12	1.81	0.62
1:J:156:PHE:CZ	1:J:161:ILE:HD13	2.34	0.62
1:O:111:LEU:H	1:O:164:GLN:HE22	1.46	0.62
1:N:148:GLN:NE2	1:N:179:CYS:H	1.94	0.61
1:O:85:CYS:HA	1:O:91:HIS:CD2	2.36	0.61
1:B:155:ASP:OD2	1:B:235:SER:HB2	2.01	0.61
1:O:102:LEU:HD23	1:O:222:ASN:HA	1.82	0.61
1:F:152:MET:HG2	1:F:153:SER:N	2.14	0.60
1:A:188:ASP:O	1:A:192:ARG:HG3	2.00	0.60
1:O:105:THR:HG21	1:O:231:PHE:HZ	1.64	0.60
1:C:143:ILE:HG13	1:C:182:ILE:HD13	1.83	0.60
1:O:121:ASP:OD1	1:O:123:HIS:N	2.28	0.60
1:L:152:MET:HG2	1:L:153:SER:N	2.16	0.60
1:O:150:GLU:OE2	1:O:169:HIS:NE2	2.33	0.60
1:P:156:PHE:CZ	1:P:161:ILE:HD13	2.36	0.60
1:M:119:LEU:HD22	1:M:125:ARG:HA	1.82	0.60
1:P:174:ASP:O	1:P:178:HIS:HD2	1.86	0.59
1:C:134:SER:O	1:C:138:THR:OG1	2.18	0.59
1:D:85:CYS:HA	1:D:91:HIS:CD2	2.36	0.59
1:K:150:GLU:HG2	1:K:181:THR:HG21	1.85	0.59
1:P:134:SER:O	1:P:138:THR:OG1	2.19	0.59
1:F:150:GLU:N	6:F:303:CIT:O4	2.31	0.59
1:H:161:ILE:HG22	1:H:222:ASN:HB2	1.84	0.59
1:P:204:TYR:OH	1:P:207:GLY:HA2	2.03	0.59
1:G:187:MET:CE	1:G:213:THR:HG21	2.33	0.58
1:O:96:VAL:HG21	4:T:1:NAG:H83	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:85:CYS:HA	1:P:91:HIS:CD2	2.38	0.58
1:F:150:GLU:OE2	1:F:169:HIS:NE2	2.36	0.58
1:E:188:ASP:OD2	1:E:191:ARG:NH2	2.30	0.57
1:J:111:LEU:H	1:J:164:GLN:NE2	2.02	0.57
1:F:85:CYS:HA	1:F:91:HIS:CD2	2.40	0.57
1:K:151:VAL:CG2	1:K:166:ASN:HB2	2.34	0.57
1:B:183:ALA:O	1:B:187:MET:HG3	2.03	0.57
1:D:150:GLU:OE2	1:D:169:HIS:CE1	2.56	0.57
1:P:148:GLN:NE2	1:P:179:CYS:H	2.02	0.57
1:E:152:MET:HG2	1:E:153:SER:N	2.20	0.57
1:E:191:ARG:NH1	1:E:201:PRO:HG3	2.20	0.57
1:F:199:LEU:HD23	1:F:213:THR:HB	1.85	0.57
1:M:121:ASP:OD2	1:M:123:HIS:N	2.34	0.57
1:A:85:CYS:HA	1:A:91:HIS:CD2	2.40	0.56
1:I:111:LEU:H	1:I:164:GLN:NE2	2.03	0.56
1:O:163:VAL:HG13	1:O:220:ILE:HB	1.86	0.56
1:H:96:VAL:HG21	3:S:1:NAG:H83	1.87	0.56
1:K:174:ASP:O	1:K:178:HIS:HD2	1.88	0.56
1:L:133:MET:O	1:L:137:THR:HG23	2.06	0.56
1:K:150:GLU:OE1	1:K:169:HIS:NE2	2.29	0.56
1:M:167:LEU:HD22	1:M:187:MET:CE	2.35	0.56
1:B:187:MET:CE	1:B:213:THR:HG21	2.35	0.56
1:E:104:LEU:HD22	1:E:220:ILE:HG12	1.88	0.56
1:A:93:TYR:HB2	1:A:103:GLU:OE1	2.06	0.56
1:L:156:PHE:CZ	1:L:161:ILE:HD13	2.41	0.56
1:D:183:ALA:O	1:D:187:MET:HG3	2.06	0.55
1:C:121:ASP:OD2	1:C:122:ALA:N	2.40	0.55
1:N:137:THR:O	1:N:140:HIS:HD2	1.90	0.55
1:C:83:LEU:HD22	1:C:230:VAL:HG22	1.87	0.55
1:K:111:LEU:H	1:K:164:GLN:NE2	2.03	0.55
1:L:202:SER:HB3	1:L:210:CYS:O	2.05	0.55
1:O:150:GLU:HG2	1:O:181:THR:HG21	1.88	0.55
1:B:115:LYS:NZ	1:B:166:ASN:HD21	2.04	0.55
1:I:168:SER:O	1:I:174:ASP:HB3	2.07	0.55
1:I:112:LEU:H	1:I:164:GLN:HE22	1.55	0.55
1:M:148:GLN:OE1	1:M:179:CYS:N	2.39	0.55
1:O:152:MET:HG2	1:O:153:SER:N	2.21	0.55
1:O:167:LEU:HD13	1:O:187:MET:HE1	1.87	0.55
1:H:112:LEU:HD21	1:H:234:PRO:HB3	1.89	0.55
1:J:85:CYS:HA	1:J:91:HIS:CD2	2.42	0.55
1:K:200:SER:HB2	1:M:203:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:112:LEU:HD12	1:J:164:GLN:HB3	1.89	0.55
1:O:110:SER:HB3	1:O:217:TYR:CZ	2.42	0.55
1:M:112:LEU:CD2	1:M:234:PRO:HB3	2.37	0.54
1:L:123:HIS:NE2	1:L:127:LEU:HD11	2.23	0.54
1:P:188:ASP:OD1	1:P:191:ARG:NH2	2.32	0.54
1:D:156:PHE:CZ	1:D:161:ILE:HD13	2.42	0.54
1:L:188:ASP:HA	1:L:211:ILE:HD11	1.89	0.54
1:E:150:GLU:HG2	1:E:181:THR:HG21	1.90	0.54
1:I:121:ASP:OD1	1:I:122:ALA:N	2.41	0.54
1:B:143:ILE:HG13	1:B:182:ILE:HD13	1.90	0.53
1:B:112:LEU:H	1:B:164:GLN:HE22	1.56	0.53
1:L:121:ASP:OD2	1:L:123:HIS:N	2.35	0.53
1:L:233:ARG:HG2	1:L:234:PRO:HD2	1.89	0.53
1:I:126:ASN:ND2	1:L:206:SER:OG	2.36	0.53
1:G:184:ASN:ND2	1:G:211:ILE:H	2.04	0.53
1:N:145:ASN:N	1:P:129:ASP:OD2	2.37	0.53
1:D:172:TYR:CE2	1:D:202:SER:O	2.62	0.53
1:F:110:SER:HB3	1:F:217:TYR:CE1	2.44	0.53
1:B:111:LEU:H	1:B:164:GLN:NE2	2.07	0.53
1:L:188:ASP:O	1:L:192:ARG:HG3	2.09	0.53
1:G:152:MET:HG2	1:G:153:SER:N	2.23	0.53
1:H:183:ALA:O	1:H:187:MET:HG3	2.09	0.53
1:O:191:ARG:NH2	1:O:192:ARG:HE	2.06	0.53
1:N:191:ARG:HG2	1:N:199:LEU:HB2	1.91	0.52
1:O:111:LEU:HG	1:O:219:ILE:HD13	1.91	0.52
1:O:96:VAL:CG2	1:O:97:ARG:N	2.72	0.52
1:A:112:LEU:H	1:A:164:GLN:HE22	1.55	0.52
1:D:187:MET:CE	1:D:213:THR:HG21	2.39	0.52
1:C:200:SER:OG	1:F:203:GLU:OE1	2.26	0.52
1:L:110:SER:HB2	1:L:164:GLN:HE22	1.73	0.52
1:D:155:ASP:OD2	1:D:156:PHE:N	2.42	0.52
1:E:150:GLU:OE2	1:E:169:HIS:NE2	2.41	0.52
1:M:183:ALA:O	1:M:187:MET:HG3	2.09	0.52
1:N:206:SER:OG	1:P:126:ASN:ND2	2.43	0.52
1:D:187:MET:HE1	1:D:213:THR:HG21	1.91	0.52
1:B:85:CYS:HA	1:B:91:HIS:CD2	2.45	0.52
1:J:139:PHE:HB2	1:J:141:LEU:HG	1.91	0.52
1:B:111:LEU:HD11	1:B:231:PHE:CD1	2.45	0.52
1:N:152:MET:HG2	1:N:153:SER:N	2.24	0.52
1:P:201:PRO:HB3	1:P:209:THR:CG2	2.40	0.52
1:I:81:MET:HE3	1:I:233:ARG:HG2	1.85	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:151:VAL:HG23	1:K:166:ASN:HB2	1.92	0.52
1:P:144:PRO:HB2	1:P:146:PHE:CE2	2.45	0.52
1:G:110:SER:HB3	1:G:217:TYR:CZ	2.45	0.51
1:H:152:MET:HG2	1:H:153:SER:N	2.25	0.51
1:K:110:SER:HB3	1:K:217:TYR:CZ	2.45	0.51
1:H:204:TYR:CE1	1:H:209:THR:HG22	2.44	0.51
1:I:126:ASN:HB2	1:L:205:ILE:HD11	1.92	0.51
1:F:96:VAL:HG23	1:F:97:ARG:HG3	1.91	0.51
1:G:187:MET:HE1	1:G:213:THR:HG21	1.93	0.51
1:I:152:MET:HG2	1:I:153:SER:N	2.25	0.51
1:K:163:VAL:CG1	1:K:220:ILE:HB	2.39	0.51
1:B:96:VAL:HG21	2:Q:1:NAG:H83	1.92	0.51
1:J:125:ARG:HG2	1:K:146:PHE:CD2	2.45	0.51
1:O:100:THR:HG21	4:T:1:NAG:HN2	1.76	0.51
1:M:121:ASP:OD2	1:M:122:ALA:N	2.44	0.51
1:P:233:ARG:HG3	1:P:234:PRO:HD2	1.93	0.51
1:K:152:MET:HG2	1:K:153:SER:N	2.26	0.51
1:D:162:THR:HG23	1:D:221:GLN:HG2	1.93	0.50
1:P:132:LEU:O	1:P:136:VAL:HG23	2.12	0.50
1:M:115:LYS:O	1:M:115:LYS:HG2	2.11	0.50
1:P:148:GLN:NE2	1:P:180:GLY:H	2.08	0.50
1:K:111:LEU:H	1:K:164:GLN:HE22	1.58	0.50
1:A:172:TYR:OH	1:A:203:GLU:OE1	2.09	0.50
1:H:110:SER:HB2	1:H:164:GLN:HE22	1.77	0.50
1:N:114:HIS:C	1:N:115:LYS:HD3	2.32	0.50
1:D:152:MET:HG2	1:D:153:SER:N	2.27	0.49
1:L:163:VAL:HB	1:L:220:ILE:HB	1.94	0.49
1:O:167:LEU:HD13	1:O:187:MET:CE	2.42	0.49
1:N:137:THR:O	1:N:140:HIS:CD2	2.65	0.49
1:F:150:GLU:HG2	1:F:181:THR:HG21	1.94	0.49
1:D:111:LEU:HD11	1:D:231:PHE:CD1	2.47	0.49
1:G:110:SER:HB2	1:G:164:GLN:HE22	1.77	0.49
1:B:133:MET:O	1:B:137:THR:HG23	2.12	0.49
1:M:83:LEU:HD21	1:P:225:TRP:CH2	2.48	0.49
1:G:155:ASP:OD1	1:G:235:SER:HB2	2.13	0.49
1:H:152:MET:HB2	1:H:165:TYR:CD2	2.47	0.49
1:I:111:LEU:H	1:I:164:GLN:HE22	1.61	0.49
1:C:169:HIS:O	1:C:212:GLN:HG2	2.13	0.48
1:I:119:LEU:HB3	1:I:125:ARG:HG2	1.94	0.48
1:B:115:LYS:HA	1:B:153:SER:OG	2.13	0.48
1:B:156:PHE:CZ	1:B:161:ILE:HD13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:GLU:HG2	1:D:181:THR:HG21	1.94	0.48
1:E:94:ILE:HG23	1:E:138:THR:HG21	1.95	0.48
1:G:96:VAL:HG23	1:G:97:ARG:HG2	1.96	0.48
1:J:226:GLU:CD	1:J:226:GLU:H	2.17	0.48
1:D:203:GLU:HG3	1:G:201:PRO:O	2.12	0.48
1:L:126:ASN:HD21	1:L:130:LYS:HZ3	1.60	0.48
1:P:150:GLU:OE2	1:P:169:HIS:NE2	2.40	0.48
1:G:167:LEU:HD13	1:G:187:MET:HE1	1.95	0.48
1:I:136:VAL:HA	1:I:141:LEU:HD12	1.96	0.48
1:P:152:MET:HG2	1:P:153:SER:N	2.27	0.48
1:C:93:TYR:HE1	1:C:95:GLN:HG3	1.77	0.48
1:P:191:ARG:NH1	1:P:201:PRO:HG3	2.28	0.48
1:H:187:MET:CE	1:H:213:THR:HG21	2.43	0.48
1:J:155:ASP:OD2	1:J:156:PHE:N	2.47	0.48
1:K:98:ASN:OD1	1:K:99:ASP:N	2.46	0.48
1:E:98:ASN:OD1	1:E:99:ASP:N	2.46	0.48
1:J:111:LEU:H	1:J:164:GLN:HE22	1.61	0.48
1:N:161:ILE:HG22	1:N:222:ASN:HB2	1.96	0.48
1:P:162:THR:HG21	1:P:234:PRO:HA	1.96	0.48
1:B:115:LYS:HZ2	1:B:166:ASN:HD21	1.62	0.47
1:D:102:LEU:HD23	1:D:222:ASN:HA	1.95	0.47
1:L:191:ARG:NH2	1:L:192:ARG:HD3	2.29	0.47
1:O:111:LEU:N	1:O:164:GLN:HE22	2.11	0.47
1:I:116:PHE:HB3	1:I:118:ASN:OD1	2.14	0.47
1:B:114:HIS:HB2	1:B:116:PHE:HD1	1.77	0.47
1:B:96:VAL:HG23	1:B:97:ARG:HG2	1.96	0.47
1:D:146:PHE:HE2	1:H:129:ASP:HB2	1.79	0.47
1:J:150:GLU:OE2	1:J:169:HIS:NE2	2.41	0.47
1:I:156:PHE:CZ	1:I:161:ILE:HD13	2.49	0.47
1:A:221:GLN:HE22	1:A:231:PHE:HA	1.80	0.47
1:B:202:SER:HB3	1:B:210:CYS:O	2.14	0.47
1:M:136:VAL:HG13	1:M:141:LEU:HB2	1.96	0.47
1:F:104:LEU:HD22	1:F:220:ILE:HG12	1.97	0.47
1:O:163:VAL:CG1	1:O:220:ILE:HB	2.44	0.47
1:L:169:HIS:O	1:L:212:GLN:HG2	2.14	0.47
1:O:105:THR:HG21	1:O:231:PHE:CZ	2.49	0.47
1:K:96:VAL:HG23	1:K:97:ARG:HG2	1.98	0.46
1:N:163:VAL:HG13	1:N:220:ILE:HB	1.97	0.46
1:O:223:THR:OG1	1:O:224:THR:N	2.47	0.46
1:P:154:CYS:HB2	1:P:161:ILE:HD11	1.98	0.46
1:H:152:MET:HB2	1:H:165:TYR:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:156:PHE:CZ	1:M:161:ILE:HD12	2.51	0.46
1:D:146:PHE:CE2	1:H:129:ASP:HB2	2.50	0.46
1:E:188:ASP:O	1:E:192:ARG:HG3	2.15	0.46
1:N:110:SER:HB3	1:N:217:TYR:CZ	2.50	0.46
1:I:119:LEU:O	1:I:125:ARG:HG3	2.16	0.46
1:P:110:SER:HB3	1:P:217:TYR:CE2	2.51	0.46
1:A:199:LEU:HD23	1:A:213:THR:HB	1.97	0.46
1:C:183:ALA:O	1:C:187:MET:HG3	2.16	0.46
1:O:121:ASP:CG	1:O:123:HIS:H	2.14	0.46
1:C:155:ASP:OD2	1:C:235:SER:HB2	2.15	0.45
1:N:163:VAL:CG1	1:N:220:ILE:HB	2.46	0.45
1:C:172:TYR:CZ	1:F:201:PRO:HG2	2.51	0.45
1:M:172:TYR:CE2	1:M:202:SER:O	2.69	0.45
1:D:121:ASP:OD2	1:D:122:ALA:N	2.50	0.45
1:H:85:CYS:HA	1:H:91:HIS:CD2	2.51	0.45
1:H:169:HIS:O	1:H:212:GLN:HG2	2.16	0.45
1:L:155:ASP:OD1	1:L:235:SER:HB2	2.16	0.45
1:F:105:THR:HG21	1:F:231:PHE:CZ	2.51	0.45
1:L:155:ASP:OD2	1:L:156:PHE:N	2.49	0.45
1:A:205:ILE:HG22	1:A:206:SER:OG	2.17	0.45
1:A:112:LEU:HD12	1:A:164:GLN:HB3	1.99	0.44
1:E:110:SER:HB3	1:E:217:TYR:CZ	2.52	0.44
1:M:111:LEU:HD11	1:M:231:PHE:CD2	2.52	0.44
1:O:116:PHE:HB3	1:O:118:ASN:OD1	2.17	0.44
1:P:160:LYS:HZ3	1:P:222:ASN:HB3	1.82	0.44
1:A:98:ASN:OD1	1:A:99:ASP:N	2.51	0.44
1:J:168:SER:O	1:J:174:ASP:HB3	2.16	0.44
1:L:126:ASN:HD21	1:L:130:LYS:HZ2	1.65	0.44
1:M:104:LEU:HD21	1:M:135:ILE:HD13	1.98	0.44
1:O:148:GLN:NE2	1:O:180:GLY:H	2.15	0.44
1:E:184:ASN:HA	1:E:187:MET:HE2	1.98	0.44
1:J:100:THR:CG2	5:J:301:NAG:HN2	2.25	0.44
1:P:144:PRO:HB2	1:P:146:PHE:CZ	2.53	0.44
1:P:160:LYS:NZ	1:P:222:ASN:C	2.70	0.44
1:B:221:GLN:HE22	1:B:231:PHE:HA	1.82	0.44
1:D:148:GLN:OE1	1:D:179:CYS:N	2.50	0.44
1:E:172:TYR:C	1:E:172:TYR:CD2	2.90	0.44
1:G:155:ASP:CG	1:G:235:SER:HB2	2.37	0.44
1:I:85:CYS:HA	1:I:91:HIS:NE2	2.33	0.44
1:J:227:ASP:OD1	1:J:227:ASP:N	2.50	0.44
1:N:150:GLU:HG2	1:N:181:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:119:LEU:HB3	1:O:125:ARG:HG2	2.00	0.44
1:I:225:TRP:CZ3	1:I:228:HIS:CE1	3.06	0.44
1:P:150:GLU:HG2	1:P:181:THR:HG21	2.00	0.44
1:I:108:ASN:OD1	1:I:216:GLN:HG3	2.17	0.44
1:K:161:ILE:HG22	1:K:222:ASN:HB2	2.00	0.44
1:L:111:LEU:HD21	1:L:231:PHE:CD2	2.53	0.44
1:N:104:LEU:HD22	1:N:220:ILE:HG12	2.00	0.44
1:O:108:ASN:OD1	1:O:216:GLN:HG3	2.18	0.44
1:M:199:LEU:HD23	1:M:213:THR:HB	1.99	0.44
1:E:107:THR:OG1	1:E:108:ASN:N	2.51	0.43
1:A:96:VAL:HG21	5:A:302:NAG:H83	1.99	0.43
1:G:81:MET:HG2	1:G:231:PHE:O	2.17	0.43
1:I:150:GLU:HG2	1:I:181:THR:HG21	1.99	0.43
1:J:112:LEU:H	1:J:164:GLN:HE22	1.66	0.43
1:H:204:TYR:CD1	1:H:209:THR:HG22	2.53	0.43
1:C:136:VAL:HA	1:C:141:LEU:HD12	2.01	0.43
1:D:110:SER:HB3	1:D:217:TYR:CZ	2.53	0.43
1:E:85:CYS:HA	1:E:91:HIS:CD2	2.53	0.43
1:F:169:HIS:ND1	1:F:211:ILE:O	2.52	0.43
1:H:188:ASP:O	1:H:192:ARG:HG3	2.18	0.43
1:H:162:THR:HG23	1:H:221:GLN:HG2	2.00	0.43
1:M:115:LYS:HE3	1:M:116:PHE:HE1	1.83	0.43
1:P:110:SER:HB2	1:P:164:GLN:HE22	1.83	0.43
1:N:172:TYR:C	1:N:172:TYR:CD1	2.92	0.43
1:P:221:GLN:NE2	1:P:231:PHE:HD1	2.16	0.43
1:G:164:GLN:HE21	1:G:166:ASN:HD21	1.67	0.43
1:O:85:CYS:HA	1:O:91:HIS:NE2	2.34	0.43
1:P:97:ARG:CG	1:P:98:ASN:H	2.22	0.43
1:D:169:HIS:HD2	1:D:211:ILE:O	2.01	0.43
1:A:111:LEU:H	1:A:164:GLN:NE2	2.17	0.42
1:D:146:PHE:CD2	1:H:125:ARG:HG2	2.54	0.42
1:L:93:TYR:HB2	1:L:103:GLU:OE2	2.19	0.42
1:O:81:MET:HE3	1:O:233:ARG:HG3	2.01	0.42
1:N:155:ASP:OD1	1:N:156:PHE:N	2.52	0.42
1:O:112:LEU:HD12	1:O:164:GLN:HB3	2.01	0.42
1:A:94:ILE:O	1:A:94:ILE:HG13	2.19	0.42
1:J:134:SER:O	1:J:138:THR:OG1	2.25	0.42
1:C:115:LYS:HD3	1:C:115:LYS:HA	1.79	0.42
1:L:167:LEU:HD21	1:L:218:LEU:HB3	2.02	0.42
1:C:112:LEU:HD12	1:C:164:GLN:HB3	2.01	0.42
1:H:104:LEU:HG	1:H:220:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:110:SER:HB3	1:I:217:TYR:CZ	2.55	0.42
1:O:148:GLN:NE2	1:O:179:CYS:H	2.12	0.42
1:A:104:LEU:HD23	1:A:186:ILE:HD13	2.01	0.42
1:C:94:ILE:HG23	1:C:138:THR:HG21	2.02	0.42
1:D:93:TYR:HB2	1:D:103:GLU:OE1	2.19	0.42
1:G:155:ASP:OD2	1:G:156:PHE:N	2.51	0.42
1:G:223:THR:OG1	1:G:224:THR:N	2.53	0.42
1:A:169:HIS:O	1:A:212:GLN:HG2	2.20	0.42
1:G:183:ALA:O	1:G:187:MET:HG3	2.20	0.42
1:N:128:TYR:CE2	1:N:132:LEU:HD11	2.54	0.41
1:H:148:GLN:OE1	1:H:179:CYS:N	2.52	0.41
1:I:134:SER:O	1:I:138:THR:OG1	2.22	0.41
1:N:148:GLN:NE2	1:N:179:CYS:N	2.66	0.41
1:N:203:GLU:HG2	1:N:205:ILE:HG12	2.03	0.41
1:O:159:GLY:O	4:T:1:NAG:O6	2.35	0.41
1:J:159:GLY:O	5:J:301:NAG:O6	2.38	0.41
1:G:81:MET:HG3	1:G:82:PRO:HD2	2.02	0.41
1:H:110:SER:HB3	1:H:217:TYR:CZ	2.55	0.41
1:O:172:TYR:CD2	1:O:172:TYR:C	2.94	0.41
1:P:160:LYS:HZ1	1:P:222:ASN:HD22	1.68	0.41
1:E:96:VAL:HG23	1:E:97:ARG:HG3	2.03	0.41
1:F:100:THR:HG22	1:F:101:GLY:N	2.36	0.41
1:G:150:GLU:OE2	1:G:169:HIS:CE1	2.74	0.41
1:J:110:SER:HB3	1:J:217:TYR:CZ	2.56	0.41
1:M:115:LYS:HE3	1:M:116:PHE:CE1	2.55	0.41
1:F:183:ALA:O	1:F:187:MET:HG3	2.21	0.41
1:C:110:SER:HB2	1:C:164:GLN:HE22	1.85	0.41
1:J:111:LEU:HD11	1:J:231:PHE:CG	2.55	0.41
1:M:136:VAL:HA	1:M:141:LEU:HD12	2.03	0.41
1:B:167:LEU:HD13	1:B:187:MET:HE3	2.02	0.41
1:L:119:LEU:HD22	1:L:125:ARG:HA	2.01	0.41
1:P:160:LYS:HZ1	1:P:222:ASN:C	2.24	0.41
1:A:111:LEU:HD21	1:A:231:PHE:CD2	2.56	0.40
1:A:135:ILE:HG21	1:A:186:ILE:HD11	2.03	0.40
1:H:121:ASP:OD2	1:H:122:ALA:N	2.54	0.40
1:H:187:MET:HE1	1:H:213:THR:HG21	2.03	0.40
1:N:204:TYR:O	1:N:205:ILE:HD13	2.22	0.40
1:P:106:LEU:HD23	1:P:218:LEU:HB2	2.03	0.40
3:S:2:NAG:O3	3:S:3:MAN:H2	2.22	0.40
1:B:119:LEU:HD22	1:B:125:ARG:HA	2.03	0.40
1:C:104:LEU:N	1:C:104:LEU:HD12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:GLN:HG3	1:D:219:ILE:HG12	2.03	0.40
1:D:98:ASN:OD1	1:D:99:ASP:N	2.54	0.40
1:L:106:LEU:HD21	1:L:187:MET:HG2	2.02	0.40
1:B:121:ASP:OD2	1:B:122:ALA:N	2.54	0.40
1:A:223:THR:OG1	1:A:224:THR:N	2.54	0.40
1:E:223:THR:OG1	1:E:224:THR:N	2.54	0.40
1:M:94:ILE:HG23	1:M:138:THR:HG21	2.02	0.40
1:N:199:LEU:HD23	1:N:213:THR:HB	2.04	0.40
1:E:83:LEU:HD23	1:E:230:VAL:HG22	2.04	0.40
1:G:85:CYS:HA	1:G:91:HIS:CD2	2.57	0.40
1:J:192:ARG:HH11	1:J:192:ARG:HD2	1.74	0.40
1:K:104:LEU:N	1:K:104:LEU:HD12	2.36	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	154/171 (90%)	151 (98%)	3 (2%)	0	100	100
1	B	154/171 (90%)	149 (97%)	5 (3%)	0	100	100
1	C	154/171 (90%)	150 (97%)	4 (3%)	0	100	100
1	D	154/171 (90%)	150 (97%)	4 (3%)	0	100	100
1	E	154/171 (90%)	150 (97%)	4 (3%)	0	100	100
1	F	154/171 (90%)	149 (97%)	5 (3%)	0	100	100
1	G	154/171 (90%)	149 (97%)	5 (3%)	0	100	100
1	H	154/171 (90%)	150 (97%)	4 (3%)	0	100	100
1	I	154/171 (90%)	151 (98%)	3 (2%)	0	100	100
1	J	154/171 (90%)	150 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	154/171 (90%)	151 (98%)	3 (2%)	0	100	100
1	L	154/171 (90%)	151 (98%)	3 (2%)	0	100	100
1	M	154/171 (90%)	150 (97%)	4 (3%)	0	100	100
1	N	154/171 (90%)	151 (98%)	3 (2%)	0	100	100
1	O	154/171 (90%)	150 (97%)	4 (3%)	0	100	100
1	P	154/171 (90%)	151 (98%)	3 (2%)	0	100	100
All	All	2464/2736 (90%)	2403 (98%)	61 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	143/154 (93%)	143 (100%)	0	100	100
1	B	143/154 (93%)	141 (99%)	2 (1%)	67	84
1	C	143/154 (93%)	141 (99%)	2 (1%)	67	84
1	D	143/154 (93%)	141 (99%)	2 (1%)	67	84
1	E	143/154 (93%)	140 (98%)	3 (2%)	53	76
1	F	143/154 (93%)	141 (99%)	2 (1%)	67	84
1	G	143/154 (93%)	142 (99%)	1 (1%)	84	93
1	H	143/154 (93%)	141 (99%)	2 (1%)	67	84
1	I	143/154 (93%)	140 (98%)	3 (2%)	53	76
1	J	143/154 (93%)	141 (99%)	2 (1%)	67	84
1	K	143/154 (93%)	140 (98%)	3 (2%)	53	76
1	L	143/154 (93%)	142 (99%)	1 (1%)	84	93
1	M	143/154 (93%)	141 (99%)	2 (1%)	67	84
1	N	143/154 (93%)	141 (99%)	2 (1%)	67	84
1	O	143/154 (93%)	141 (99%)	2 (1%)	67	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	143/154 (93%)	141 (99%)	2 (1%)	67	84
All	All	2288/2464 (93%)	2257 (99%)	31 (1%)	67	84

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	80	THR
1	B	118	ASN
1	C	109	THR
1	C	115	LYS
1	D	172	TYR
1	D	233	ARG
1	E	109	THR
1	E	130	LYS
1	E	148	GLN
1	F	113	ASP
1	F	115	LYS
1	G	150	GLU
1	H	138	THR
1	H	200	SER
1	I	87	LYS
1	I	120	SER
1	I	163	VAL
1	J	115	LYS
1	J	142	ASN
1	K	113	ASP
1	K	148	GLN
1	K	212	GLN
1	L	211	ILE
1	M	148	GLN
1	M	172	TYR
1	N	113	ASP
1	N	174	ASP
1	O	113	ASP
1	O	212	GLN
1	P	80	THR
1	P	222	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	88	ASN
1	B	89	ASN
1	B	166	ASN
1	B	197	ASN
1	B	216	GLN
1	B	221	GLN
1	A	164	GLN
1	A	178	HIS
1	A	197	ASN
1	A	221	GLN
1	C	88	ASN
1	C	177	ASN
1	D	142	ASN
1	D	164	GLN
1	D	169	HIS
1	D	178	HIS
1	D	221	GLN
1	E	95	GLN
1	E	118	ASN
1	F	212	GLN
1	F	221	GLN
1	G	88	ASN
1	G	95	GLN
1	G	123	HIS
1	G	166	ASN
1	G	169	HIS
1	G	177	ASN
1	G	178	HIS
1	G	184	ASN
1	G	221	GLN
1	H	88	ASN
1	H	95	GLN
1	H	216	GLN
1	I	126	ASN
1	I	147	ASN
1	I	164	GLN
1	I	212	GLN
1	I	221	GLN
1	J	89	ASN
1	J	142	ASN
1	J	164	GLN
1	J	212	GLN
1	K	88	ASN

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Mol	Chain	Res	Type
1	K	164	GLN
1	K	166	ASN
1	K	178	HIS
1	K	212	GLN
1	K	221	GLN
1	L	95	GLN
1	L	126	ASN
1	L	147	ASN
1	L	212	GLN
1	M	88	ASN
1	M	98	ASN
1	M	178	HIS
1	N	140	HIS
1	N	148	GLN
1	N	197	ASN
1	O	88	ASN
1	O	126	ASN
1	O	148	GLN
1	O	164	GLN
1	O	166	ASN
1	P	89	ASN
1	P	92	HIS
1	P	95	GLN
1	P	98	ASN
1	P	126	ASN
1	P	148	GLN
1	P	178	HIS
1	P	222	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 ⓘ

13 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$
2	NAG	Q	1	1,2	14,14,15	0.40	0	17,19,21	1.83	2 (11%)
2	NAG	Q	2	2	14,14,15	0.59	0	17,19,21	0.61	0
2	NAG	R	1	1,2	14,14,15	0.27	0	17,19,21	1.02	2 (11%)
2	NAG	R	2	2	14,14,15	1.26	1 (7%)	17,19,21	1.17	1 (5%)
3	NAG	S	1	1,3	14,14,15	0.25	0	17,19,21	0.53	0
3	NAG	S	2	3	14,14,15	0.27	0	17,19,21	0.43	0
3	MAN	S	3	3	11,11,12	0.99	1 (9%)	15,15,17	1.16	2 (13%)
3	MAN	S	4	3	11,11,12	1.03	1 (9%)	15,15,17	2.53	2 (13%)
4	NAG	T	1	1,4	14,14,15	0.30	0	17,19,21	0.38	0
4	NAG	T	2	4	14,14,15	0.43	0	17,19,21	0.64	0
4	MAN	T	3	4	11,11,12	1.14	2 (18%)	15,15,17	1.16	2 (13%)
4	MAN	T	4	4	11,11,12	1.64	3 (27%)	15,15,17	1.30	2 (13%)
4	MAN	T	5	4	11,11,12	1.05	0	15,15,17	0.91	1 (6%)

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
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	MAN	S	3	3	-	2/2/19/22	0/1/1/1
3	MAN	S	4	3	-	1/2/19/22	0/1/1/1
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	1/6/23/26	0/1/1/1
4	MAN	T	3	4	-	2/2/19/22	0/1/1/1
4	MAN	T	4	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	T	5	4	-	1/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	2	NAG	O5-C1	4.37	1.50	1.43
4	T	4	MAN	C2-C3	3.25	1.57	1.52
4	T	4	MAN	O2-C2	2.82	1.49	1.43
3	S	4	MAN	O5-C5	2.51	1.48	1.43
4	T	3	MAN	C2-C3	2.31	1.55	1.52
3	S	3	MAN	C4-C3	2.30	1.58	1.52
4	T	3	MAN	O5-C1	-2.18	1.40	1.43
4	T	4	MAN	C1-C2	2.02	1.56	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	4	MAN	C1-O5-C5	8.37	123.53	112.19
2	Q	1	NAG	C1-O5-C5	4.97	118.92	112.19
2	Q	1	NAG	O4-C4-C5	4.88	121.41	109.30
2	R	2	NAG	C1-O5-C5	4.57	118.38	112.19
3	S	4	MAN	O5-C1-C2	3.90	116.79	110.77
4	T	4	MAN	O2-C2-C1	3.28	115.86	109.15
2	R	1	NAG	C1-O5-C5	2.78	115.96	112.19
3	S	3	MAN	C1-O5-C5	2.41	115.45	112.19
2	R	1	NAG	O4-C4-C5	-2.38	103.39	109.30
3	S	3	MAN	O2-C2-C3	-2.37	105.39	110.14
4	T	3	MAN	C1-O5-C5	2.21	115.18	112.19
4	T	3	MAN	O2-C2-C3	-2.20	105.73	110.14
4	T	5	MAN	O2-C2-C3	-2.17	105.79	110.14
4	T	4	MAN	C1-C2-C3	2.03	112.16	109.67

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	R	1	NAG	O5-C5-C6-O6
3	S	3	MAN	O5-C5-C6-O6
4	T	3	MAN	O5-C5-C6-O6
3	S	3	MAN	C4-C5-C6-O6
4	T	3	MAN	C4-C5-C6-O6

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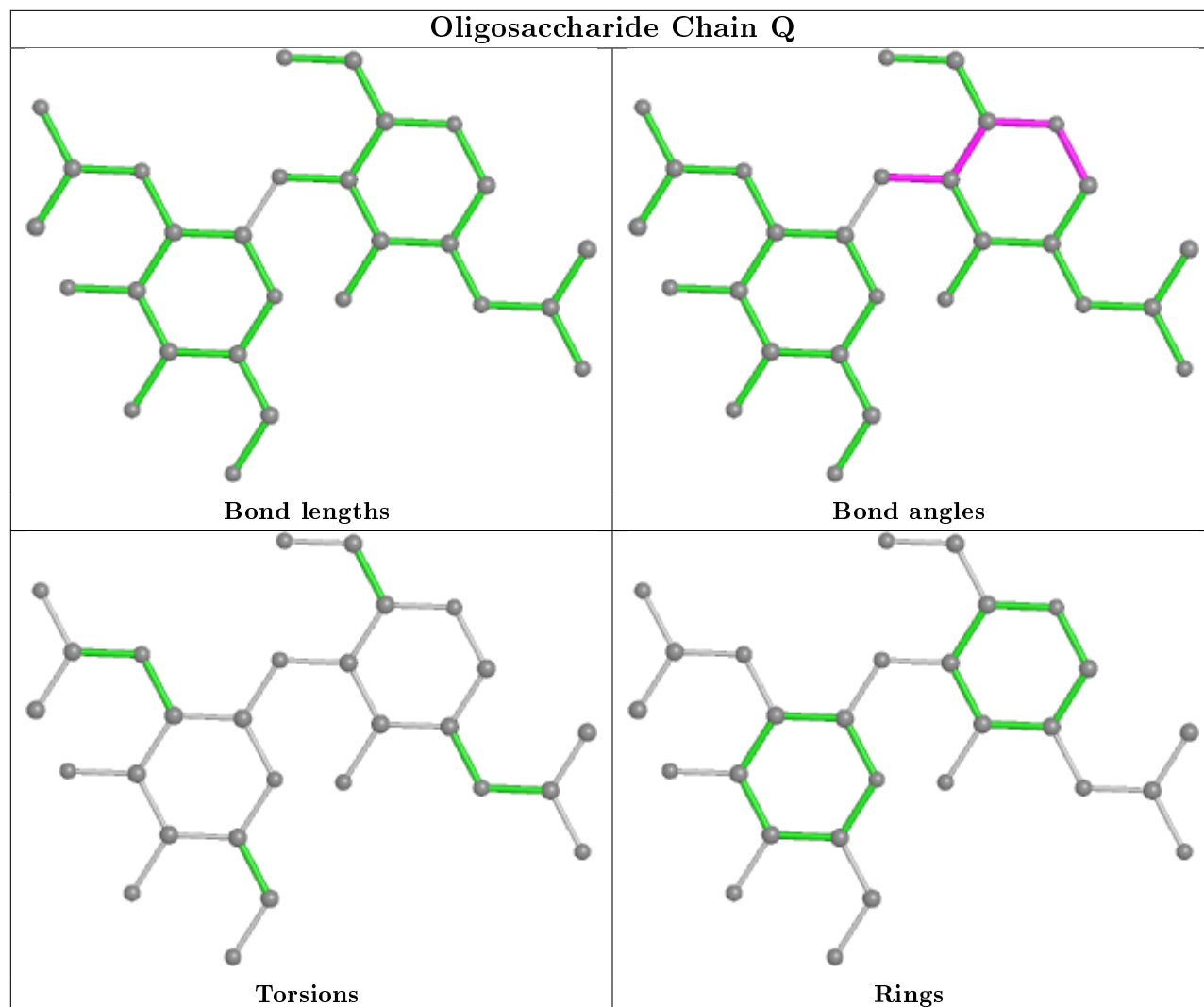
Mol	Chain	Res	Type	Atoms
4	T	1	NAG	O5-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
3	S	4	MAN	O5-C5-C6-O6
2	R	2	NAG	C1-C2-N2-C7
4	T	5	MAN	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
2	R	2	NAG	C3-C2-N2-C7

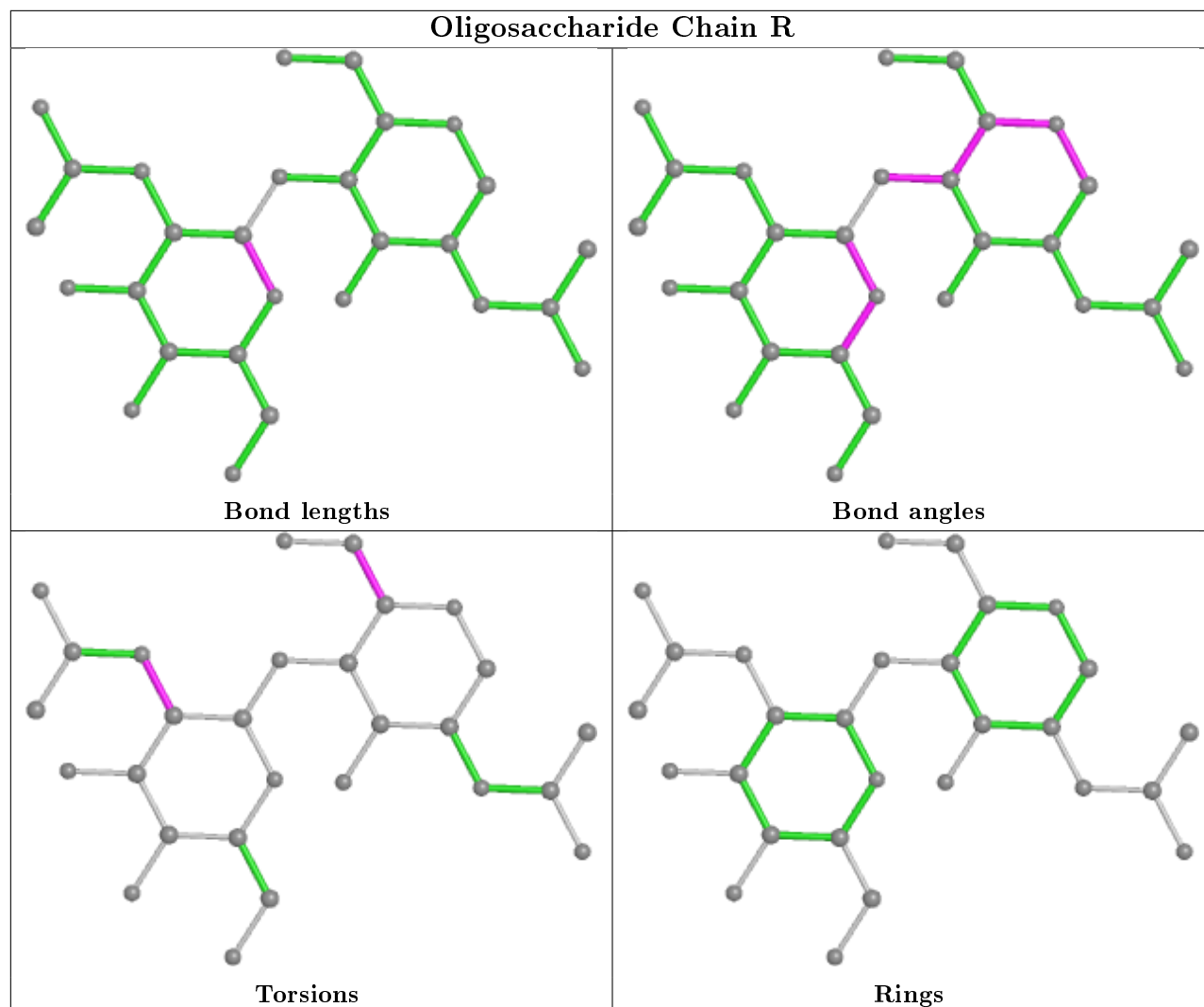
There are no ring outliers.

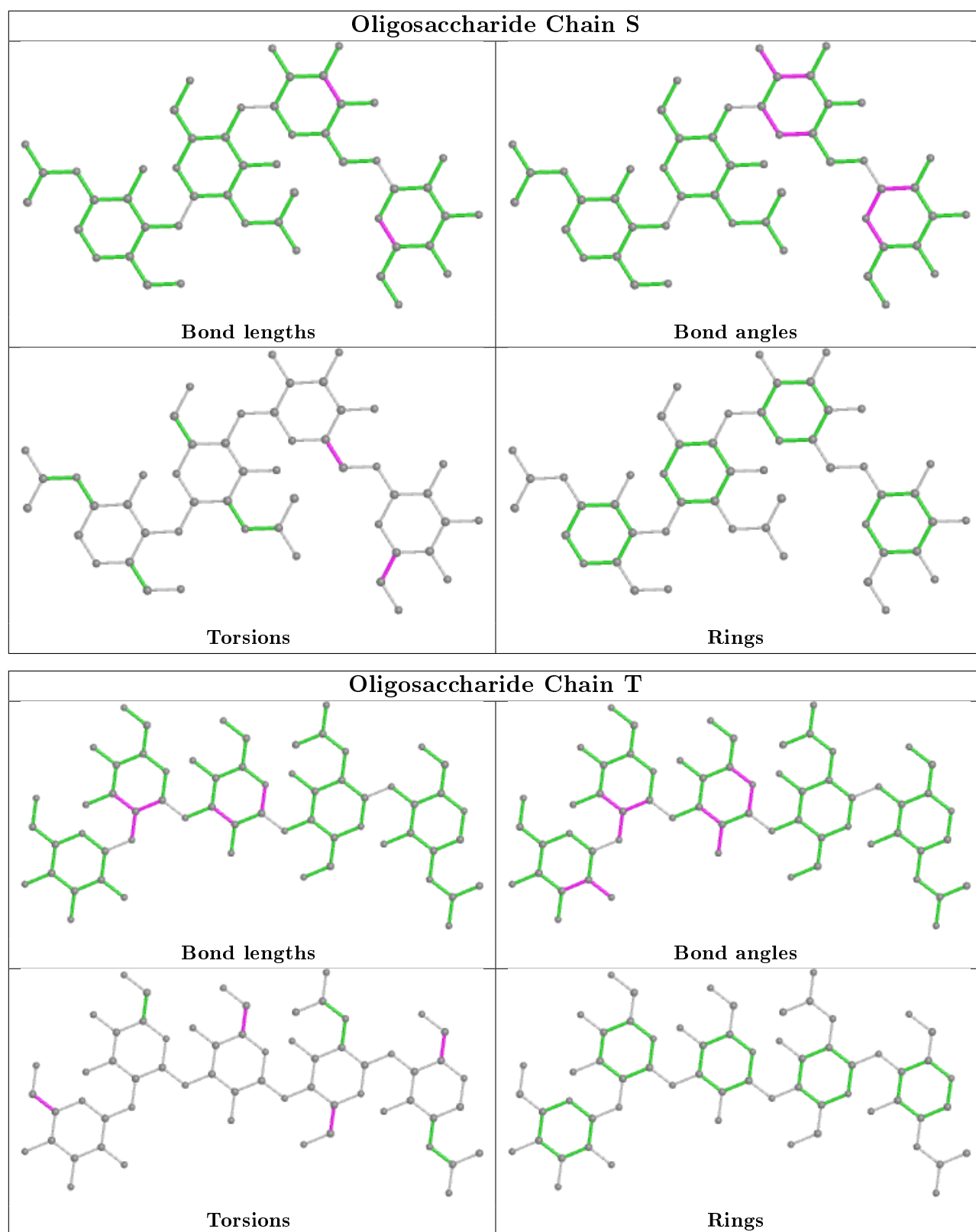
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	2	NAG	1	0
3	S	3	MAN	1	0
3	S	2	NAG	1	0
4	T	1	NAG	3	0
2	Q	1	NAG	2	0
3	S	1	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 oligosaccharide.







5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	E	301	1	14,14,15	0.37	0	17,19,21	0.58	0
5	NAG	B	301	1	14,14,15	0.54	0	17,19,21	0.98	1 (5%)
5	NAG	A	301	1	14,14,15	0.39	0	17,19,21	0.68	1 (5%)
5	NAG	G	302	1	14,14,15	0.19	0	17,19,21	0.62	0
5	NAG	K	301	1	14,14,15	0.54	0	17,19,21	0.77	1 (5%)
5	NAG	E	302	1	14,14,15	0.59	1 (7%)	17,19,21	0.52	0
5	NAG	J	301	1	14,14,15	0.48	0	17,19,21	0.64	1 (5%)
5	NAG	H	301	1	14,14,15	0.39	0	17,19,21	0.75	1 (5%)
5	NAG	G	301	1	14,14,15	0.32	0	17,19,21	0.63	1 (5%)
5	NAG	A	302	1	14,14,15	0.34	0	17,19,21	0.58	0
5	NAG	I	301	1	14,14,15	0.70	1 (7%)	17,19,21	1.33	1 (5%)
6	CIT	F	303	-	3,12,12	1.64	1 (33%)	3,17,17	3.14	2 (66%)
6	CIT	I	302	-	3,12,12	1.41	0	3,17,17	2.25	2 (66%)
6	CIT	C	303	-	3,12,12	1.84	1 (33%)	3,17,17	2.72	1 (33%)
6	CIT	B	305	-	3,12,12	1.17	0	3,17,17	2.93	1 (33%)
5	NAG	B	304	1	14,14,15	0.71	0	17,19,21	0.81	1 (5%)
6	CIT	C	302	-	3,12,12	1.34	0	3,17,17	1.97	1 (33%)
5	NAG	L	301	1	14,14,15	0.40	0	17,19,21	0.62	1 (5%)
6	CIT	E	303	-	3,12,12	1.05	0	3,17,17	2.68	2 (66%)
5	NAG	D	301	1	14,14,15	0.52	0	17,19,21	0.82	1 (5%)
5	NAG	C	301	1	14,14,15	0.25	0	17,19,21	0.72	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	301	1	-	2/6/23/26	0/1/1/1
5	NAG	B	301	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	301	1	-	2/6/23/26	0/1/1/1
5	NAG	G	302	1	-	0/6/23/26	0/1/1/1
5	NAG	K	301	1	-	2/6/23/26	0/1/1/1
5	NAG	E	302	1	-	0/6/23/26	0/1/1/1
5	NAG	J	301	1	-	3/6/23/26	0/1/1/1
5	NAG	H	301	1	-	2/6/23/26	0/1/1/1
5	NAG	G	301	1	-	2/6/23/26	0/1/1/1
5	NAG	A	302	1	-	2/6/23/26	0/1/1/1
5	NAG	I	301	1	-	2/6/23/26	0/1/1/1
6	CIT	F	303	-	-	0/6/16/16	-
6	CIT	I	302	-	-	3/6/16/16	-
6	CIT	C	303	-	-	3/6/16/16	-
6	CIT	B	305	-	-	3/6/16/16	-
5	NAG	B	304	1	-	4/6/23/26	0/1/1/1
6	CIT	C	302	-	-	4/6/16/16	-
5	NAG	L	301	1	-	2/6/23/26	0/1/1/1
6	CIT	E	303	-	-	0/6/16/16	-
5	NAG	D	301	1	-	0/6/23/26	0/1/1/1
5	NAG	C	301	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	301	NAG	O5-C1	2.45	1.47	1.43
6	C	303	CIT	C4-C3	-2.33	1.51	1.54
5	E	302	NAG	C1-C2	2.13	1.55	1.52
6	F	303	CIT	C4-C3	-2.02	1.52	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	301	NAG	C1-O5-C5	5.28	119.35	112.19
6	B	305	CIT	C3-C4-C5	-4.66	107.52	114.98
6	F	303	CIT	C3-C4-C5	-4.64	107.56	114.98
6	C	303	CIT	C3-C4-C5	-4.25	108.18	114.98
5	B	301	NAG	C1-O5-C5	3.71	117.22	112.19
6	E	303	CIT	C3-C4-C5	-3.61	109.20	114.98
5	D	301	NAG	C1-O5-C5	3.08	116.37	112.19
5	B	304	NAG	C1-O5-C5	2.94	116.17	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	302	CIT	C3-C4-C5	-2.83	110.46	114.98
5	H	301	NAG	C1-O5-C5	2.76	115.94	112.19
5	K	301	NAG	C1-O5-C5	2.72	115.87	112.19
6	C	302	CIT	C3-C4-C5	-2.69	110.68	114.98
6	E	303	CIT	C3-C2-C1	-2.60	110.82	114.98
6	F	303	CIT	C3-C2-C1	-2.56	110.89	114.98
5	C	301	NAG	C1-O5-C5	2.53	115.62	112.19
6	I	302	CIT	C3-C2-C1	-2.48	111.01	114.98
5	A	301	NAG	C1-O5-C5	2.39	115.43	112.19
5	G	301	NAG	C1-O5-C5	2.20	115.17	112.19
5	L	301	NAG	C1-O5-C5	2.17	115.13	112.19
5	J	301	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	302	CIT	C6-C3-C4-C5
6	B	305	CIT	C1-C2-C3-O7
6	B	305	CIT	C1-C2-C3-C4
6	B	305	CIT	C1-C2-C3-C6
6	C	302	CIT	C1-C2-C3-C6
5	I	301	NAG	C4-C5-C6-O6
5	B	304	NAG	C4-C5-C6-O6
5	I	301	NAG	O5-C5-C6-O6
5	H	301	NAG	C4-C5-C6-O6
5	K	301	NAG	O5-C5-C6-O6
5	B	304	NAG	O5-C5-C6-O6
5	L	301	NAG	O5-C5-C6-O6
5	A	302	NAG	O5-C5-C6-O6
5	L	301	NAG	C4-C5-C6-O6
5	K	301	NAG	C4-C5-C6-O6
5	H	301	NAG	O5-C5-C6-O6
5	G	301	NAG	O5-C5-C6-O6
5	A	302	NAG	C4-C5-C6-O6
5	J	301	NAG	C8-C7-N2-C2
5	J	301	NAG	O7-C7-N2-C2
5	G	301	NAG	C4-C5-C6-O6
5	A	301	NAG	O5-C5-C6-O6
6	I	302	CIT	O7-C3-C4-C5
5	B	304	NAG	C1-C2-N2-C7
5	A	301	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	I	302	CIT	C2-C3-C4-C5
6	C	302	CIT	C1-C2-C3-O7
6	C	302	CIT	C1-C2-C3-C4
5	J	301	NAG	O5-C5-C6-O6
6	C	303	CIT	C1-C2-C3-C6
6	C	303	CIT	C6-C3-C4-C5
6	C	302	CIT	C2-C3-C4-C5
5	B	304	NAG	C3-C2-N2-C7
5	E	301	NAG	C4-C5-C6-O6
5	E	301	NAG	O5-C5-C6-O6
6	C	303	CIT	O7-C3-C4-C5

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	301	NAG	1	0
5	G	302	NAG	1	0
5	J	301	NAG	3	0
5	A	302	NAG	1	0
6	F	303	CIT	1	0
6	C	303	CIT	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	156/171 (91%)	-0.15	3 (1%) 66 62	34, 52, 85, 102	0
1	B	156/171 (91%)	-0.14	5 (3%) 47 41	26, 44, 71, 111	0
1	C	156/171 (91%)	-0.14	2 (1%) 77 73	23, 43, 79, 111	0
1	D	156/171 (91%)	-0.08	6 (3%) 40 34	33, 52, 84, 107	0
1	E	156/171 (91%)	-0.17	2 (1%) 77 73	32, 52, 79, 103	0
1	F	156/171 (91%)	-0.14	4 (2%) 56 50	29, 46, 78, 115	0
1	G	156/171 (91%)	-0.14	1 (0%) 89 88	33, 52, 83, 104	0
1	H	156/171 (91%)	-0.14	1 (0%) 89 88	38, 55, 87, 115	0
1	I	156/171 (91%)	-0.05	3 (1%) 66 62	31, 50, 87, 130	0
1	J	156/171 (91%)	-0.10	5 (3%) 47 41	32, 50, 83, 125	0
1	K	156/171 (91%)	-0.17	4 (2%) 56 50	31, 43, 70, 100	0
1	L	156/171 (91%)	-0.03	6 (3%) 40 34	37, 53, 88, 114	0
1	M	156/171 (91%)	-0.01	7 (4%) 33 27	32, 50, 85, 125	0
1	N	156/171 (91%)	0.02	4 (2%) 56 50	42, 67, 102, 119	0
1	O	156/171 (91%)	-0.15	1 (0%) 89 88	36, 51, 78, 115	0
1	P	156/171 (91%)	0.09	10 (6%) 19 15	44, 68, 100, 135	0
All	All	2496/2736 (91%)	-0.09	64 (2%) 56 50	23, 52, 88, 135	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	97	ARG	6.4
1	H	80	THR	5.8
1	J	80	THR	4.8
1	M	80	THR	4.8
1	M	97	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	P	97	ARG	4.6
1	J	97	ARG	4.6
1	M	114	HIS	4.2
1	I	98	ASN	4.0
1	J	114	HIS	3.9
1	P	173	VAL	3.7
1	B	97	ARG	3.4
1	F	97	ARG	3.3
1	B	98	ASN	3.3
1	P	116	PHE	3.3
1	L	97	ARG	3.2
1	B	235	SER	3.1
1	P	115	LYS	3.1
1	K	97	ARG	3.1
1	D	99	ASP	3.0
1	P	177	ASN	3.0
1	N	113	ASP	3.0
1	P	174	ASP	3.0
1	F	100	THR	2.9
1	F	235	SER	2.9
1	A	116	PHE	2.8
1	J	113	ASP	2.8
1	I	116	PHE	2.8
1	L	99	ASP	2.8
1	M	235	SER	2.7
1	P	96	VAL	2.7
1	B	113	ASP	2.7
1	A	97	ARG	2.7
1	M	116	PHE	2.7
1	F	99	ASP	2.6
1	N	158	GLY	2.6
1	E	116	PHE	2.6
1	D	113	ASP	2.5
1	K	116	PHE	2.5
1	L	98	ASN	2.5
1	C	80	THR	2.5
1	L	80	THR	2.5
1	P	99	ASP	2.5
1	M	115	LYS	2.4
1	A	98	ASN	2.4
1	N	97	ARG	2.4
1	D	111	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	80	THR	2.3
1	D	100	THR	2.3
1	G	97	ARG	2.3
1	K	113	ASP	2.3
1	E	80	THR	2.2
1	O	99	ASP	2.2
1	M	233	ARG	2.2
1	J	116	PHE	2.2
1	P	98	ASN	2.2
1	B	114	HIS	2.2
1	D	233	ARG	2.2
1	C	98	ASN	2.1
1	N	114	HIS	2.1
1	K	98	ASN	2.1
1	D	235	SER	2.1
1	L	204	TYR	2.1
1	L	113	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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.

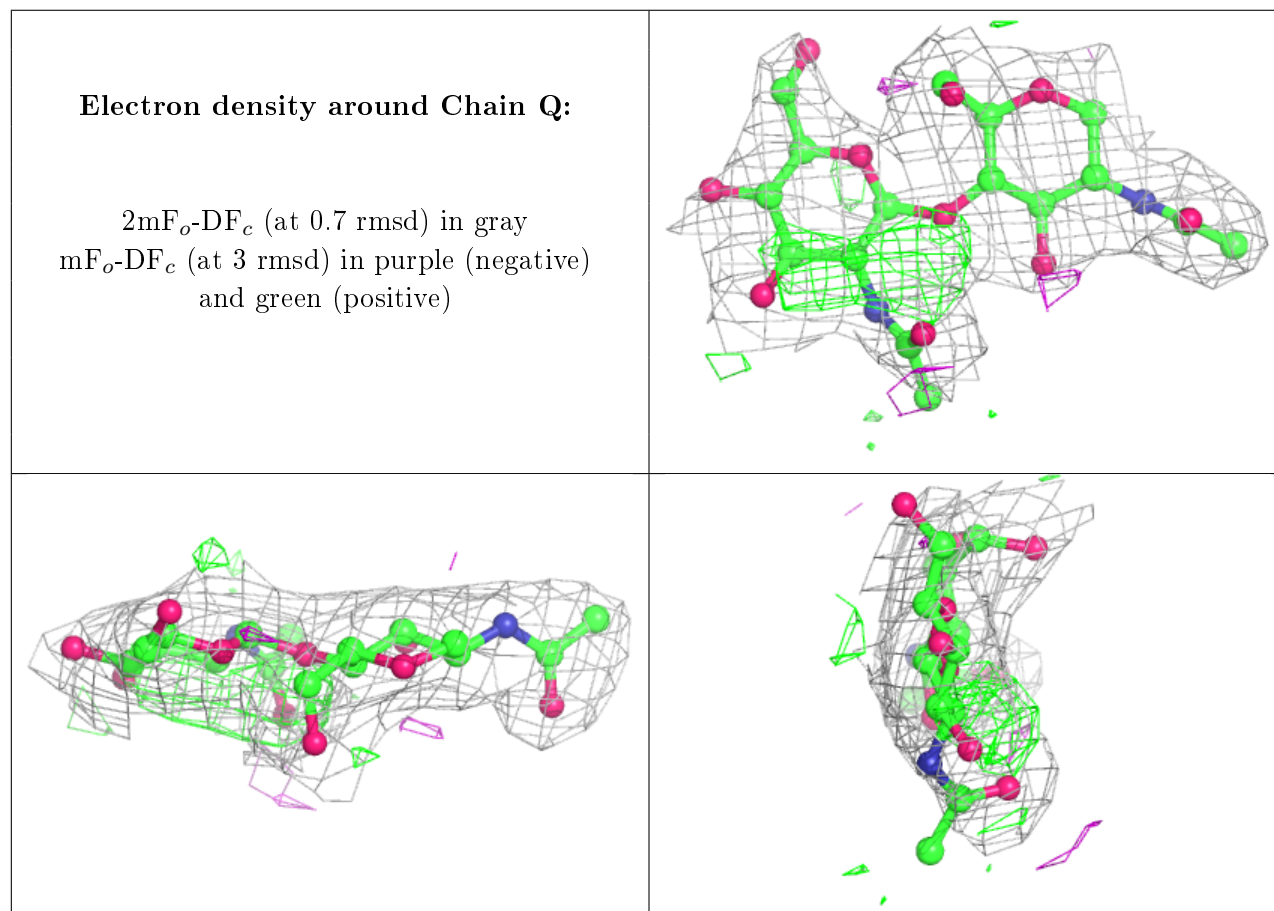
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	T	5	11/12	0.67	0.23	102,114,119,119	0
4	MAN	T	3	11/12	0.76	0.17	92,99,110,115	0
3	MAN	S	4	11/12	0.77	0.20	61,72,92,93	0
4	MAN	T	4	11/12	0.86	0.22	107,112,117,121	0
2	NAG	R	2	14/15	0.88	0.21	62,81,114,122	0
2	NAG	Q	2	14/15	0.88	0.21	65,70,88,93	0
3	MAN	S	3	11/12	0.89	0.17	58,81,99,104	0
4	NAG	T	2	14/15	0.90	0.21	89,102,113,113	0
4	NAG	T	1	14/15	0.91	0.14	44,61,66,68	0
2	NAG	R	1	14/15	0.92	0.16	39,57,70,72	0
3	NAG	S	2	14/15	0.95	0.16	51,66,75,89	0

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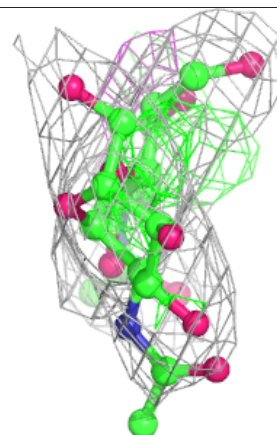
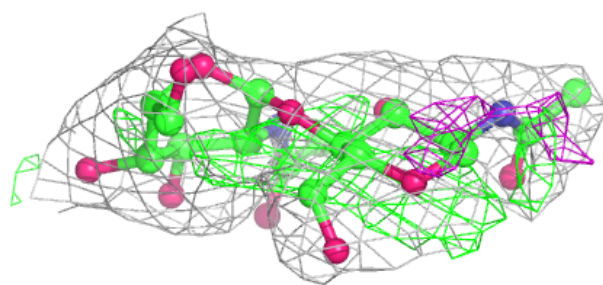
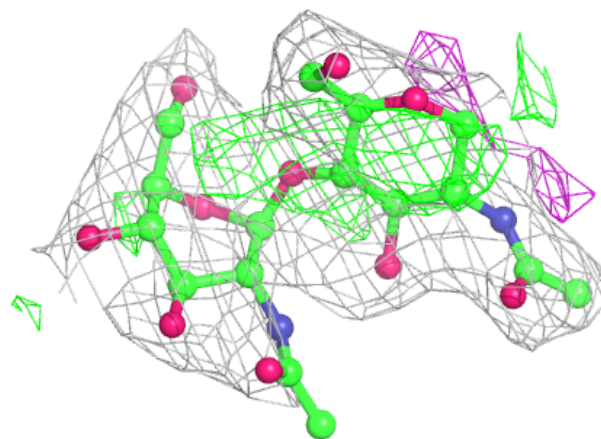
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	S	1	14/15	0.95	0.12	52,58,66,66	0
2	NAG	Q	1	14/15	0.96	0.13	37,54,57,57	0

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.

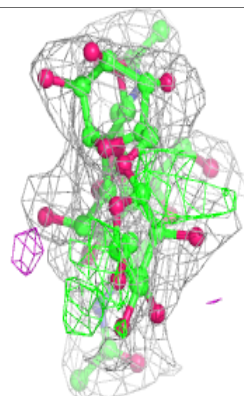
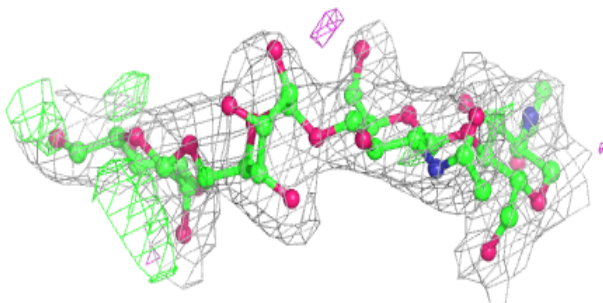
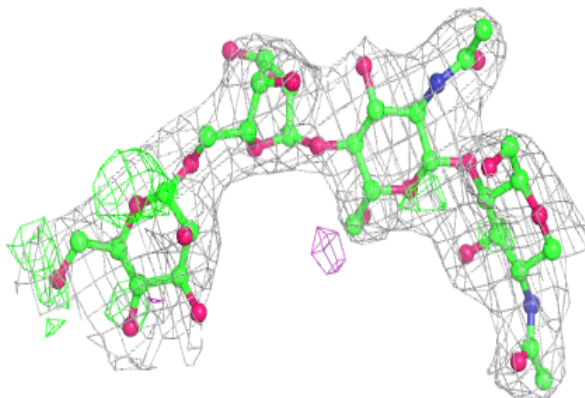


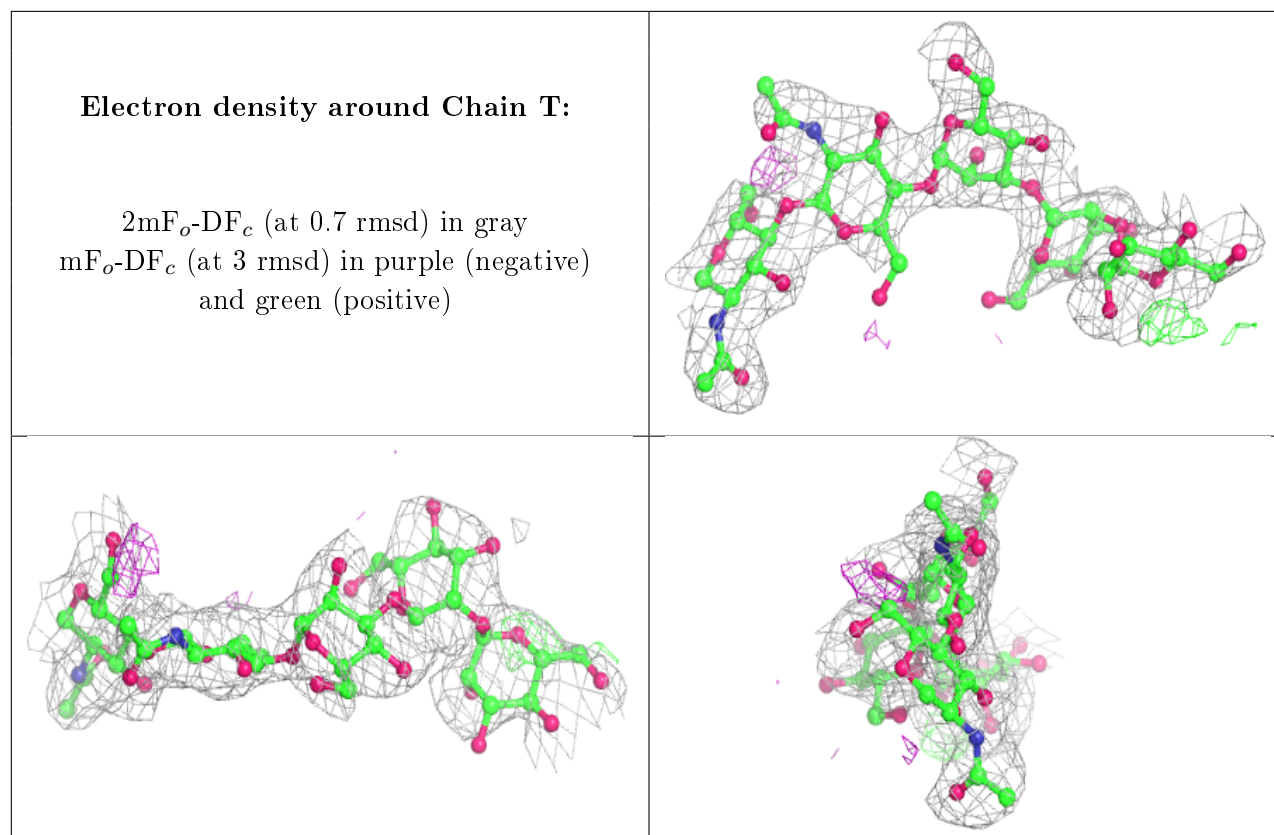
Electron density around Chain R:

$2mF_o-DF_c$ (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)





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	CIT	C	302	13/13	0.81	0.20	70,89,99,102	0
5	NAG	B	304	14/15	0.84	0.22	87,95,115,122	0
5	NAG	I	301	14/15	0.87	0.34	82,96,103,111	0
5	NAG	A	301	14/15	0.91	0.17	43,52,63,72	0
6	CIT	C	303	13/13	0.91	0.17	72,77,91,91	0
5	NAG	E	302	14/15	0.92	0.17	41,59,68,79	0
5	NAG	J	301	14/15	0.92	0.16	27,47,74,76	0
5	NAG	G	302	14/15	0.92	0.18	42,60,72,80	0
5	NAG	L	301	14/15	0.93	0.16	43,53,75,76	0
5	NAG	D	301	14/15	0.93	0.18	41,49,64,66	0
5	NAG	C	301	14/15	0.93	0.14	37,51,63,67	0
5	NAG	H	301	14/15	0.94	0.18	48,61,75,76	0
5	NAG	G	301	14/15	0.94	0.15	38,49,62,67	0
5	NAG	E	301	14/15	0.94	0.14	45,55,70,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	B	301	14/15	0.94	0.16	30,42,67,69	0
6	CIT	F	303	13/13	0.94	0.20	46,67,83,83	0
6	CIT	I	302	13/13	0.95	0.16	46,68,82,83	0
5	NAG	K	301	14/15	0.96	0.11	32,42,50,71	0
6	CIT	E	303	13/13	0.96	0.20	33,43,60,67	0
6	CIT	B	305	13/13	0.97	0.16	25,44,54,60	0
5	NAG	A	302	14/15	0.97	0.14	41,55,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.