



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 07:21 PM BST

PDB ID : 3USU
Title : Crystal structure of Butea monosperma seed lectin
Authors : Abhilash, J.; Geethanandan, K.; Bharath, S.R.; Sadasivan, C.; Haridas, M.
Deposited on : 2011-11-24
Resolution : 2.46 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

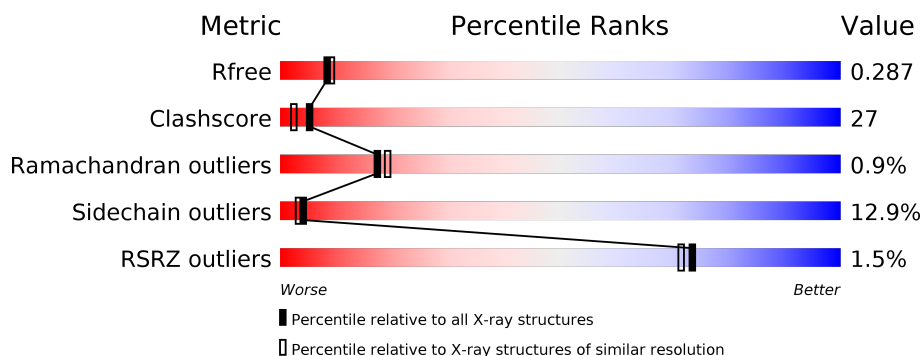
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	256	
1	C	256	
1	E	256	
1	G	256	
2	B	242	
2	D	242	

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Mol	Chain	Length	Quality of chain
2	F	242	
2	H	242	
3	I	4	
3	K	4	
3	L	4	
4	J	5	
5	M	2	
6	N	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	XYP	B	306	-	-	X	-
4	BMA	J	3	-	-	X	-
9	ABU	A	280	-	-	X	-
9	ABU	B	276	-	-	X	-
9	ABU	C	282	-	-	X	-
9	ABU	E	288	-	-	X	-
9	ABU	F	290	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 15748 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.

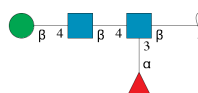
- Molecule 1 is a protein called Lectin Alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	0	0	0
			1892	1227	296	369			
1	C	250	Total	C	N	O	0	0	0
			1892	1227	296	369			
1	E	250	Total	C	N	O	0	0	0
			1892	1227	296	369			
1	G	250	Total	C	N	O	0	0	0
			1892	1227	296	369			

- Molecule 2 is a protein called Lectin Beta Chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	0	0	0
			1828	1184	287	357			
2	D	242	Total	C	N	O	0	0	0
			1828	1184	287	357			
2	F	242	Total	C	N	O	0	0	0
			1828	1184	287	357			
2	H	242	Total	C	N	O	0	0	0
			1828	1184	287	357			

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



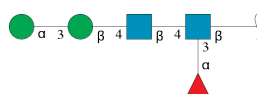
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	4	Total	C	N	O	0	0	0
			49	28	2	19			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	4	Total	C	N	O	0	0	0
			49	28	2	19			
3	L	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	5	Total	C	N	O	0	0	0
			60	34	2	24			

- 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
5	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	N	2	Total	C	N	O	0	0	0
			24	14	1	9			

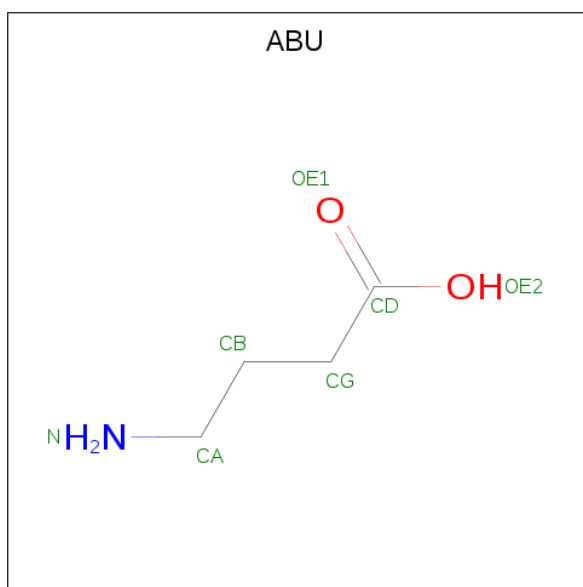
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total Ca 1 1	0	0
7	D	1	Total Ca 1 1	0	0
7	E	1	Total Ca 1 1	0	0
7	H	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0
7	A	1	Total Ca 1 1	0	0
7	F	1	Total Ca 1 1	0	0

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	1	Total Mn 1 1	0	0
8	D	1	Total Mn 1 1	0	0
8	E	1	Total Mn 1 1	0	0
8	H	1	Total Mn 1 1	0	0
8	B	1	Total Mn 1 1	0	0
8	C	1	Total Mn 1 1	0	0
8	A	1	Total Mn 1 1	0	0
8	F	1	Total Mn 1 1	0	0

- Molecule 9 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: C₄H₉NO₂).



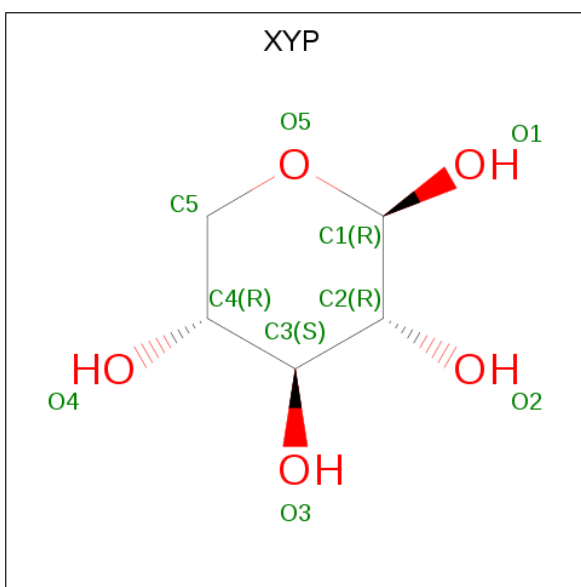
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			7	4	1	2		
9	B	1	Total	C	N	O	0	0
			7	4	1	2		
9	C	1	Total	C	N	O	0	0
			7	4	1	2		
9	D	1	Total	C	N	O	0	0
			7	4	1	2		
9	E	1	Total	C	N	O	0	0
			7	4	1	2		
9	E	1	Total	C	N	O	0	0
			7	4	1	2		
9	F	1	Total	C	N	O	0	0
			7	4	1	2		
9	G	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



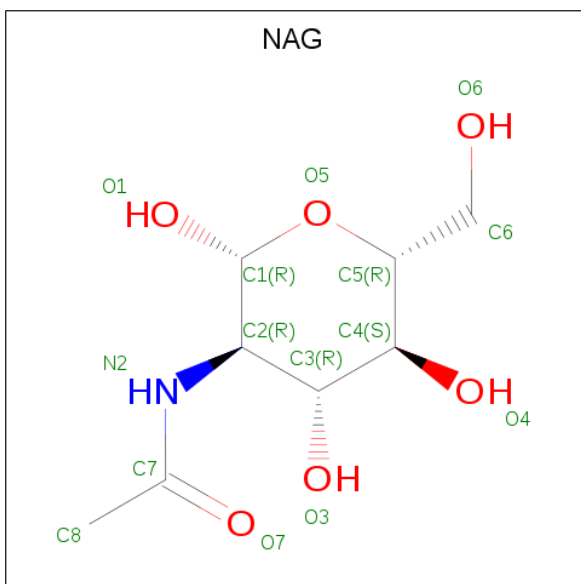
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		
10	E	1	Total	C	O	0	0
			6	3	3		
10	E	1	Total	C	O	0	0
			6	3	3		
10	G	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is beta-D-xylopyranose (three-letter code: XYP) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			9	5	4		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

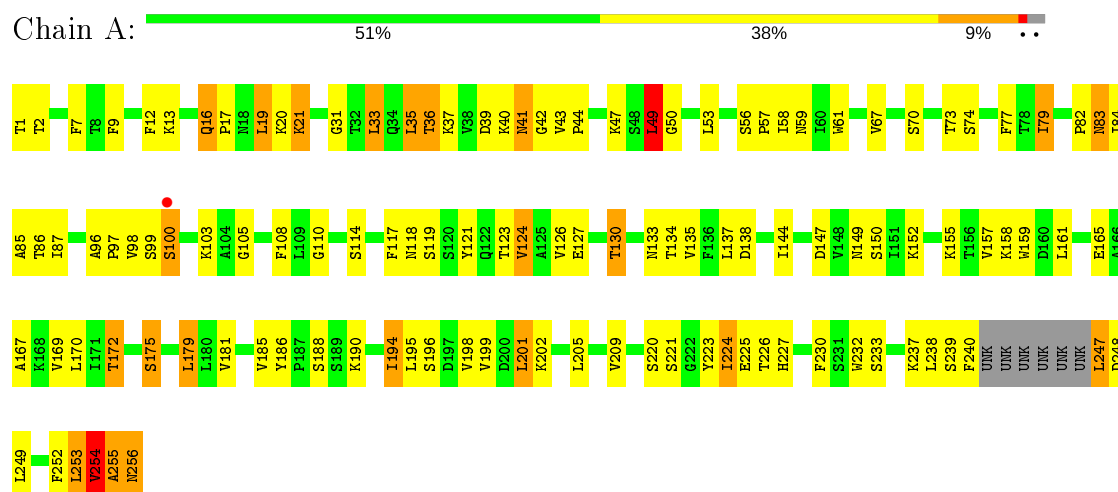
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	65	Total 65	O 65	0	0
13	B	70	Total 70	O 70	0	0
13	C	64	Total 64	O 64	0	0
13	D	47	Total 47	O 47	0	0
13	E	51	Total 51	O 51	0	0
13	F	65	Total 65	O 65	0	0
13	G	60	Total 60	O 60	0	0
13	H	44	Total 44	O 44	0	0

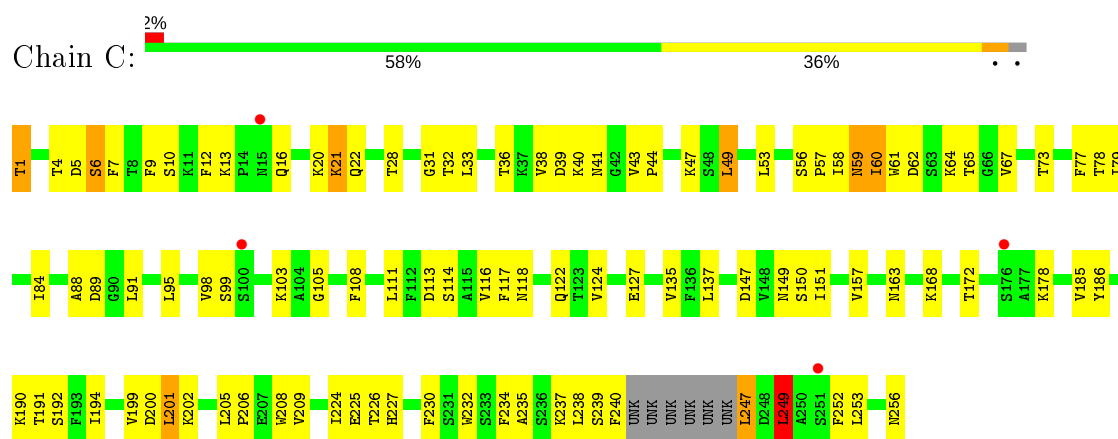
3 Residue-property plots [i](#)

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.

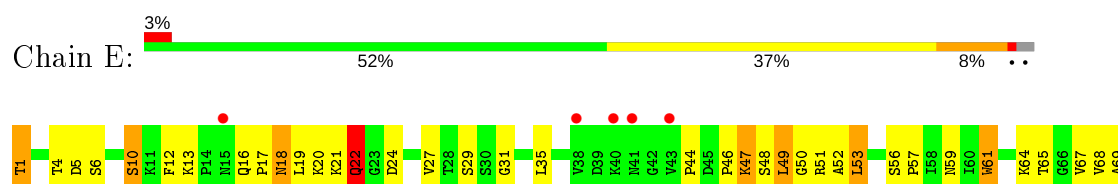
• Molecule 1: Lectin Alpha chain

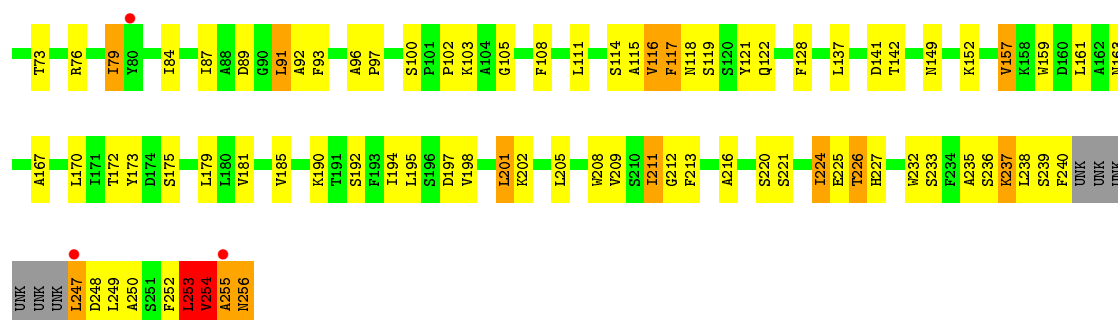


• Molecule 1: Lectin Alpha chain

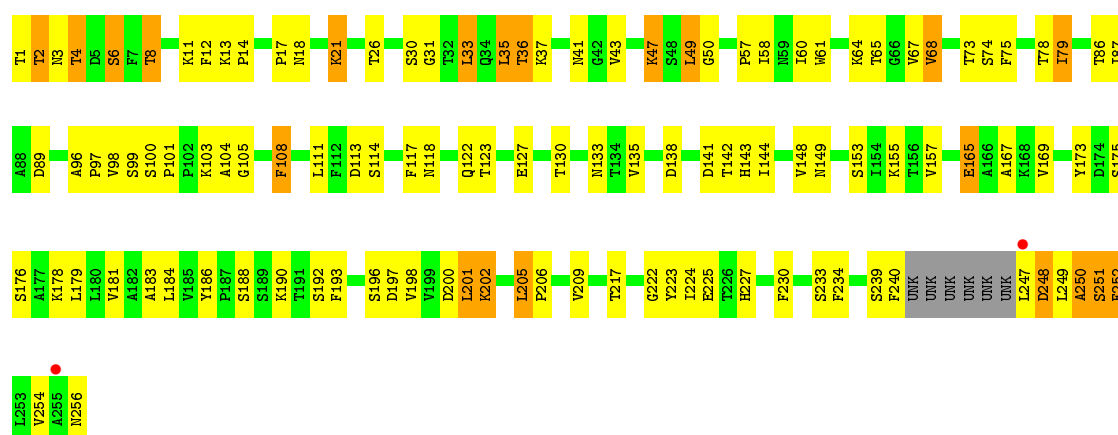


• Molecule 1: Lectin Alpha chain

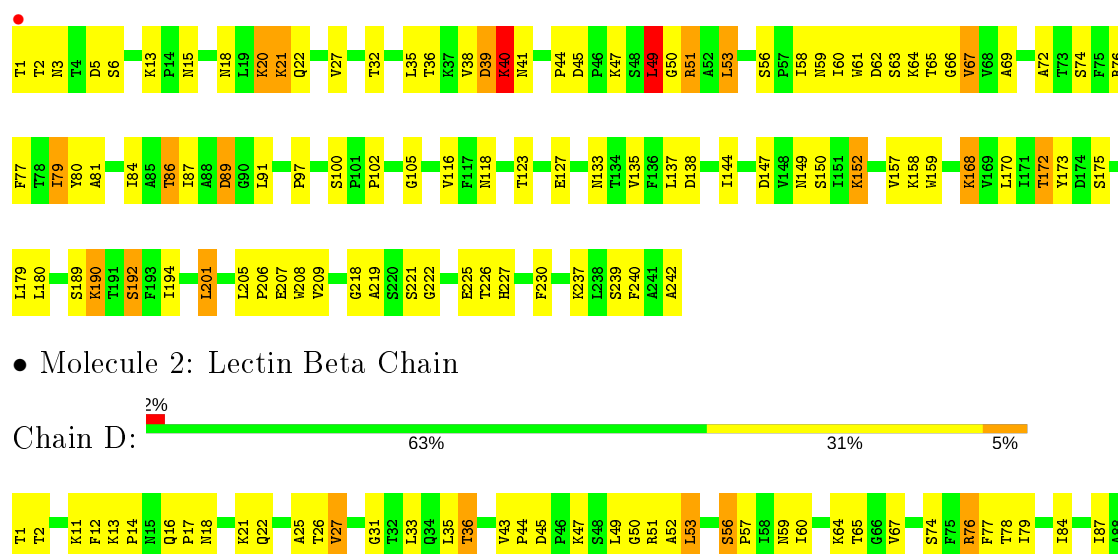




• Molecule 1: Lectin Alpha chain

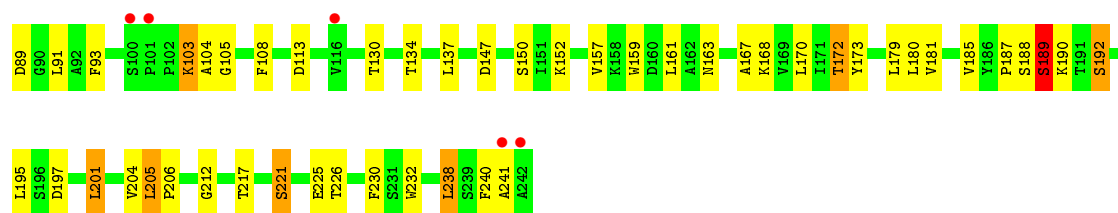


• Molecule 2: Lectin Beta Chain

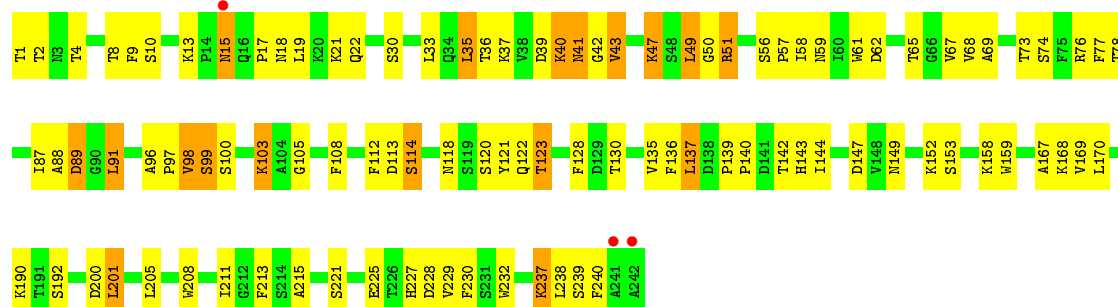


• Molecule 2: Lectin Beta Chain

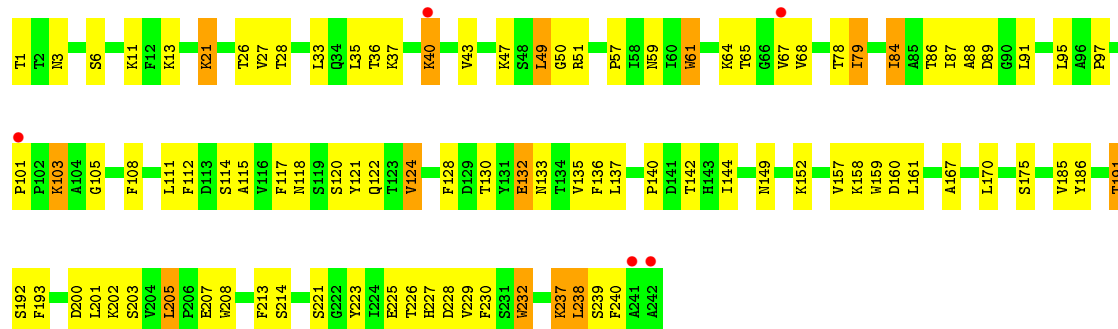




• Molecule 2: Lectin Beta Chain



• Molecule 2: Lectin Beta Chain



• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  50% 50%

MAG1
MAG2
BMA3
FUC4

- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  40% 60%

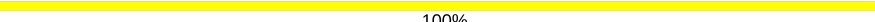
MAG1
MAG2
BMA3
MAA4
FUC5

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

Chain M:  100%

MAG1
MAG2

- Molecule 6: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.45Å 78.91Å 101.85Å 74.30° 76.65° 86.88°	Depositor
Resolution (Å)	69.06 – 2.46 69.06 – 2.46	Depositor EDS
% Data completeness (in resolution range)	94.7 (69.06-2.46) 94.7 (69.06-2.46)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.205 , 0.287 0.206 , 0.287	Depositor DCC
R_{free} test set	3944 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15748	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XYP, GOL, BMA, NAG, CA, MN, ABU, MAN, FUC

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	0.90	2/1939 (0.1%)	0.96	0/2646
1	C	0.79	3/1939 (0.2%)	0.91	1/2646 (0.0%)
1	E	0.77	2/1939 (0.1%)	0.89	3/2646 (0.1%)
1	G	0.74	1/1939 (0.1%)	0.89	0/2646
2	B	0.85	1/1875 (0.1%)	0.94	3/2560 (0.1%)
2	D	0.75	2/1875 (0.1%)	0.84	2/2560 (0.1%)
2	F	0.83	2/1875 (0.1%)	0.93	3/2560 (0.1%)
2	H	0.72	2/1875 (0.1%)	0.85	0/2560
All	All	0.80	15/15256 (0.1%)	0.90	12/20824 (0.1%)

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	A	0	1
1	C	0	1
1	E	0	1
All	All	0	3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	TRP	CD2-CE2	5.96	1.48	1.41
2	H	61	TRP	CD2-CE2	5.95	1.48	1.41
1	C	208	TRP	CD2-CE2	5.78	1.48	1.41
1	E	61	TRP	CD2-CE2	5.58	1.48	1.41
2	D	232	TRP	CD2-CE2	5.58	1.48	1.41
1	G	61	TRP	CD2-CE2	5.48	1.48	1.41
2	F	61	TRP	CD2-CE2	5.38	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	61	TRP	CD2-CE2	5.31	1.47	1.41
1	A	159	TRP	CD2-CE2	5.30	1.47	1.41
2	D	159	TRP	CD2-CE2	5.27	1.47	1.41
2	F	208	TRP	CD2-CE2	5.10	1.47	1.41
1	E	208	TRP	CD2-CE2	5.04	1.47	1.41
2	B	61	TRP	CD2-CE2	5.03	1.47	1.41
1	C	232	TRP	NE1-CE2	-5.02	1.31	1.37
2	H	232	TRP	CD2-CE2	5.01	1.47	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	39	ASP	CB-CG-OD1	7.57	125.11	118.30
1	E	253	LEU	CA-CB-CG	6.04	129.19	115.30
2	B	49	LEU	CA-CB-CG	-5.96	101.60	115.30
1	C	249	LEU	CA-CB-CG	5.89	128.84	115.30
1	E	253	LEU	CB-CG-CD2	-5.72	101.28	111.00
2	D	241	ALA	CB-CA-C	-5.65	101.63	110.10
2	B	53	LEU	CA-CB-CG	5.45	127.84	115.30
2	F	47	LYS	CD-CE-NZ	-5.33	99.44	111.70
1	E	19	LEU	CA-CB-CG	5.27	127.42	115.30
2	F	200	ASP	CB-CG-OD1	5.23	123.00	118.30
2	F	114	SER	CB-CA-C	-5.23	100.17	110.10
2	D	103	LYS	CB-CA-C	-5.09	100.21	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	VAL	Peptide
1	C	247	LEU	Peptide
1	E	22	GLN	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	1892	0	1874	128	0
1	C	1892	0	1875	97	0
1	E	1892	0	1875	112	0
1	G	1892	0	1875	114	0
2	B	1828	0	1809	108	0
2	D	1828	0	1810	80	0
2	F	1828	0	1810	96	0
2	H	1828	0	1810	112	0
3	I	49	0	43	4	0
3	K	49	0	42	0	0
3	L	49	0	43	1	0
4	J	60	0	47	9	0
5	M	28	0	25	0	0
6	N	24	0	21	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
9	A	7	0	5	5	0
9	B	7	0	5	6	0
9	C	7	0	5	6	0
9	D	7	0	5	1	0
9	E	14	0	10	11	0
9	F	7	0	5	7	0
9	G	7	0	5	1	0
10	A	6	0	8	2	0
10	B	6	0	8	0	0
10	C	6	0	8	1	0
10	D	6	0	8	0	0
10	E	12	0	16	2	0
10	G	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	6	0	8	3	0
11	B	9	0	0	6	0
12	D	14	0	12	0	0
13	A	65	0	0	16	0
13	B	70	0	0	20	0
13	C	64	0	0	13	0
13	D	47	0	0	11	0
13	E	51	0	0	5	0
13	F	65	0	0	13	0
13	G	60	0	0	17	0
13	H	44	0	0	15	0
All	All	15748	0	15075	806	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 27.

All (806) 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:H:238:LEU:HG	13:H:261:HOH:O	1.30	1.28
1:G:101:PRO:HD2	13:G:542:HOH:O	1.34	1.23
11:B:306:XYP:C1	4:J:3:BMA:O2	1.87	1.21
10:H:289:GOL:H2	13:H:411:HOH:O	1.45	1.15
1:A:36:THR:HG21	1:A:227:HIS:HD2	1.04	1.13
1:A:67:VAL:HG11	1:A:239:SER:O	1.47	1.13
2:B:40:LYS:H	2:B:40:LYS:HD3	1.02	1.13
1:E:254:VAL:HG12	1:E:255:ALA:N	1.58	1.13
1:C:59:ASN:H	9:C:282:ABU:HE2	1.15	1.10
1:C:157:VAL:HG22	13:C:321:HOH:O	1.51	1.09
1:E:59:ASN:H	9:E:284:ABU:HB2	1.13	1.07
2:H:67:VAL:HG21	2:H:239:SER:O	1.55	1.05
1:E:254:VAL:HG12	1:E:255:ALA:H	1.08	1.05
1:E:93:PHE:CE1	1:E:211:ILE:HD11	1.91	1.04
2:H:84:ILE:H	2:H:84:ILE:HD12	1.22	1.03
1:A:252:PHE:O	1:A:256:ASN:HB2	1.57	1.03
2:D:36:THR:HG22	13:D:253:HOH:O	1.57	1.03
2:F:49:LEU:HD21	2:F:105:GLY:HA2	1.39	1.01
1:G:49:LEU:HD21	1:G:105:GLY:HA3	1.39	1.01
1:A:56:SER:HB2	13:D:289:HOH:O	1.60	1.00
1:E:252:PHE:HD2	1:E:253:LEU:H	1.04	1.00
1:G:100:SER:HA	13:G:542:HOH:O	1.62	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:ASP:OD2	1:C:65:THR:HG22	1.59	1.00
10:A:277:GOL:H11	2:B:172:THR:HG21	1.40	0.99
1:E:44:PRO:HG2	1:E:224:ILE:HG23	1.43	0.99
1:A:36:THR:HG21	1:A:227:HIS:CD2	1.97	0.99
2:H:117:PHE:HZ	13:H:386:HOH:O	1.47	0.98
2:B:168:LYS:HE3	13:B:429:HOH:O	1.62	0.97
1:C:67:VAL:HG11	1:C:239:SER:O	1.65	0.97
1:E:67:VAL:HG21	1:E:239:SER:O	1.64	0.96
2:F:56:SER:HB2	13:G:547:HOH:O	1.64	0.96
1:E:252:PHE:CD2	1:E:253:LEU:N	2.33	0.95
1:A:124:VAL:HG23	13:A:297:HOH:O	1.65	0.95
2:F:40:LYS:HG2	13:F:373:HOH:O	1.64	0.95
2:B:40:LYS:H	2:B:40:LYS:CD	1.72	0.95
9:E:288:ABU:HG2	2:H:3:ASN:ND2	1.83	0.94
2:D:65:THR:OG1	2:D:67:VAL:HG22	1.66	0.94
2:B:67:VAL:HG21	2:B:239:SER:O	1.66	0.93
1:G:248:ASP:OD2	1:G:251:SER:HB2	1.67	0.93
1:E:252:PHE:O	1:E:256:ASN:HB2	1.68	0.92
2:F:9:PHE:HE1	2:F:18:ASN:HD22	1.17	0.92
1:E:254:VAL:CG1	1:E:255:ALA:N	2.29	0.92
1:E:47:LYS:HB3	1:E:47:LYS:NZ	1.85	0.91
1:G:36:THR:HG23	13:G:559:HOH:O	1.70	0.91
2:H:118:ASN:O	2:H:149:ASN:HB3	1.69	0.91
2:D:201:LEU:HG	2:D:205:LEU:HD22	1.53	0.91
2:H:67:VAL:HG11	2:H:240:PHE:HA	1.51	0.90
2:F:59:ASN:ND2	1:G:13:LYS:HZ2	1.70	0.90
2:B:49:LEU:HD11	2:B:105:GLY:HA2	1.53	0.90
1:G:47:LYS:NZ	1:G:47:LYS:HB3	1.85	0.90
1:A:172:THR:HG23	13:A:275:HOH:O	1.71	0.89
2:B:49:LEU:HD11	2:B:105:GLY:CA	2.02	0.89
1:C:28:THR:HG22	1:C:32:THR:H	1.38	0.88
1:E:252:PHE:HD2	1:E:253:LEU:N	1.71	0.88
1:A:36:THR:CG2	1:A:227:HIS:HD2	1.86	0.88
2:H:36:THR:OG1	2:H:227:HIS:HD2	1.56	0.88
2:D:230:PHE:HD2	13:D:244:HOH:O	1.56	0.87
1:A:67:VAL:HG13	13:A:291:HOH:O	1.75	0.87
1:A:254:VAL:O	1:A:255:ALA:HB2	1.74	0.86
2:B:40:LYS:N	2:B:40:LYS:HD3	1.76	0.85
1:C:59:ASN:N	9:C:282:ABU:HE2	1.90	0.85
1:C:185:VAL:HG11	2:D:179:LEU:HD21	1.57	0.85
2:H:40:LYS:H	2:H:40:LYS:HD3	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:ILE:CD1	1:G:225:GLU:HB2	2.04	0.85
2:H:40:LYS:HD3	2:H:40:LYS:N	1.91	0.84
2:F:67:VAL:HG21	2:F:239:SER:O	1.78	0.83
2:F:65:THR:OG1	2:F:67:VAL:HG12	1.77	0.83
1:A:59:ASN:H	9:A:280:ABU:HE2	1.43	0.83
1:A:39:ASP:OD2	1:A:41:ASN:HB2	1.78	0.83
1:C:4:THR:HG23	13:C:259:HOH:O	1.76	0.83
1:E:59:ASN:N	9:E:284:ABU:HB2	1.92	0.82
2:H:1:THR:O	2:H:240:PHE:HD1	1.62	0.82
2:H:105:GLY:O	2:H:108:PHE:HD2	1.61	0.82
2:D:137:LEU:HD23	2:D:152:LYS:HD2	1.61	0.81
1:G:49:LEU:HD21	1:G:105:GLY:CA	2.11	0.81
2:D:188:SER:O	2:D:189:SER:HB3	1.80	0.81
2:B:59:ASN:H	9:B:276:ABU:HB2	1.46	0.81
1:C:118:ASN:O	1:C:149:ASN:HB3	1.79	0.81
1:C:20:LYS:HE2	1:C:22:GLN:HG2	1.63	0.81
1:C:201:LEU:HD22	1:C:205:LEU:HD12	1.63	0.80
11:B:306:XYP:C1	4:J:3:BMA:C2	2.59	0.80
1:A:254:VAL:CG1	1:A:254:VAL:O	2.30	0.80
1:A:230:PHE:HD1	13:A:567:HOH:O	1.65	0.80
2:F:15:ASN:HB2	13:F:268:HOH:O	1.80	0.80
1:E:22:GLN:HE22	1:E:51:ARG:HH11	1.28	0.80
2:B:36:THR:OG1	2:B:227:HIS:HD2	1.65	0.79
2:D:221:SER:HA	13:D:257:HOH:O	1.80	0.79
1:A:124:VAL:CG2	13:A:297:HOH:O	2.28	0.79
1:A:157:VAL:HG22	13:A:259:HOH:O	1.80	0.79
2:F:4:THR:HG22	2:F:237:LYS:HB2	1.63	0.79
1:E:93:PHE:HE1	1:E:211:ILE:HD11	1.42	0.79
2:F:123:THR:HG21	13:F:561:HOH:O	1.82	0.79
2:D:67:VAL:HG21	2:D:240:PHE:HA	1.64	0.79
2:H:67:VAL:HG13	2:H:238:LEU:HD21	1.64	0.79
1:E:93:PHE:CZ	1:E:211:ILE:HD11	2.18	0.78
1:G:47:LYS:HZ3	1:G:47:LYS:HB3	1.47	0.78
1:C:247:LEU:HD23	1:C:247:LEU:N	1.97	0.78
1:C:28:THR:HG22	1:C:32:THR:N	1.98	0.78
1:E:157:VAL:HG22	1:E:195:LEU:HB2	1.64	0.78
9:F:290:ABU:N	1:G:18:ASN:HD22	1.80	0.78
1:C:201:LEU:HD22	1:C:205:LEU:CD1	2.14	0.77
2:D:36:THR:HG21	2:D:217:THR:HG23	1.65	0.77
1:A:49:LEU:HD11	1:A:105:GLY:CA	2.15	0.77
2:B:172:THR:HG23	13:B:250:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:58:ILE:HA	9:F:290:ABU:CA	2.13	0.76
1:C:28:THR:CG2	1:C:32:THR:H	1.98	0.76
1:E:47:LYS:HB3	1:E:47:LYS:HZ2	1.50	0.76
2:B:86:THR:O	2:B:86:THR:HG22	1.83	0.76
2:D:33:LEU:HG	2:D:35:LEU:HD12	1.68	0.76
2:H:84:ILE:HD12	2:H:84:ILE:N	1.99	0.76
1:E:253:LEU:HD21	2:F:170:LEU:HD21	1.65	0.76
1:G:201:LEU:HG	1:G:205:LEU:HD22	1.67	0.75
1:E:118:ASN:O	1:E:149:ASN:HB3	1.86	0.75
1:E:172:THR:HG21	1:E:249:LEU:HD11	1.67	0.75
1:G:179:LEU:CD1	13:G:290:HOH:O	2.32	0.75
2:H:40:LYS:H	2:H:40:LYS:CD	2.00	0.75
2:B:207:GLU:HG2	13:B:256:HOH:O	1.87	0.75
1:E:22:GLN:NE2	1:E:51:ARG:HH11	1.85	0.74
13:F:258:HOH:O	1:G:4:THR:CG2	2.36	0.74
2:B:67:VAL:HG11	2:B:240:PHE:HA	1.68	0.74
2:F:140:PRO:HD2	13:F:391:HOH:O	1.88	0.74
2:D:35:LEU:O	2:D:50:GLY:HA3	1.86	0.74
2:F:108:PHE:HE1	2:F:114:SER:HA	1.52	0.74
13:F:258:HOH:O	1:G:4:THR:HG23	1.88	0.74
1:C:230:PHE:HD1	13:C:494:HOH:O	1.70	0.73
2:F:9:PHE:HE1	2:F:18:ASN:ND2	1.86	0.73
2:B:1:THR:O	2:B:1:THR:HG22	1.87	0.73
1:A:79:ILE:HD13	1:A:225:GLU:HB2	1.70	0.73
11:B:306:XYP:C2	4:J:3:BMA:O2	2.36	0.73
13:F:258:HOH:O	1:G:6:SER:HB2	1.88	0.72
1:A:36:THR:HG23	13:A:395:HOH:O	1.90	0.72
1:C:200:ASP:O	1:C:201:LEU:HB2	1.89	0.72
1:A:44:PRO:HG2	1:A:224:ILE:HG23	1.71	0.72
1:E:1:THR:HG22	1:E:240:PHE:HD2	1.55	0.72
2:H:84:ILE:H	2:H:84:ILE:CD1	1.98	0.72
2:H:87:ILE:HG13	2:H:130:THR:HG22	1.71	0.72
2:B:201:LEU:HG	2:B:205:LEU:HD12	1.71	0.72
10:A:277:GOL:C1	2:B:172:THR:HG21	2.19	0.71
1:A:67:VAL:CG1	1:A:239:SER:O	2.34	0.71
1:G:103:LYS:HB3	1:G:113:ASP:OD1	1.89	0.71
1:A:1:THR:O	1:A:240:PHE:HD2	1.73	0.71
2:B:63:SER:N	13:B:256:HOH:O	2.22	0.71
1:C:1:THR:HG23	1:C:240:PHE:HB2	1.71	0.71
1:E:1:THR:HG22	1:E:240:PHE:CD2	2.25	0.71
1:E:198:VAL:HG22	2:F:190:LYS:HE3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:CD1	1:A:225:GLU:HB2	2.21	0.70
1:C:247:LEU:N	13:C:284:HOH:O	2.23	0.70
1:E:201:LEU:HG	1:E:205:LEU:HD12	1.73	0.70
1:C:79:ILE:HD11	1:C:91:LEU:HD22	1.73	0.70
1:A:19:LEU:HD12	1:A:21:LYS:HZ1	1.57	0.70
1:E:22:GLN:HE22	1:E:51:ARG:NH1	1.88	0.70
2:F:49:LEU:HD21	2:F:105:GLY:CA	2.20	0.70
1:A:49:LEU:HD11	1:A:105:GLY:HA2	1.72	0.69
2:B:18:ASN:HD22	9:C:282:ABU:N	1.88	0.69
1:C:194:ILE:HG23	2:D:192:SER:HB3	1.74	0.69
1:C:58:ILE:HD13	9:C:282:ABU:CA	2.23	0.69
2:H:185:VAL:HG22	2:H:192:SER:HB3	1.74	0.69
2:F:152:LYS:HE3	13:F:277:HOH:O	1.92	0.69
1:G:36:THR:CG2	13:G:559:HOH:O	2.34	0.69
2:B:135:VAL:HG12	13:B:271:HOH:O	1.93	0.69
1:C:44:PRO:HG3	1:C:226:THR:HG23	1.75	0.69
1:A:253:LEU:C	1:A:255:ALA:H	1.95	0.69
1:G:33:LEU:HD22	1:G:35:LEU:HD13	1.73	0.69
2:B:62:ASP:HA	13:B:256:HOH:O	1.93	0.69
2:D:56:SER:HB3	13:D:289:HOH:O	1.91	0.69
2:H:157:VAL:HG22	13:H:254:HOH:O	1.91	0.69
2:F:59:ASN:HD21	1:G:13:LYS:HZ2	1.38	0.69
13:A:381:HOH:O	2:B:237:LYS:HD3	1.92	0.69
1:G:21:LYS:HB2	1:G:21:LYS:HZ2	1.58	0.69
1:E:254:VAL:C	1:E:256:ASN:H	1.97	0.68
1:G:68:VAL:HG22	1:G:175:SER:HB2	1.74	0.68
2:F:108:PHE:CE1	2:F:114:SER:HA	2.28	0.68
2:F:59:ASN:HD21	1:G:13:LYS:NZ	1.90	0.68
2:H:36:THR:OG1	2:H:227:HIS:CD2	2.45	0.68
3:I:2:NAG:H61	3:I:4:FUC:H3	1.75	0.68
2:H:225:GLU:OE2	2:H:227:HIS:HE1	1.77	0.68
1:C:65:THR:HG23	1:C:67:VAL:H	1.59	0.68
2:B:239:SER:OG	2:B:242:ALA:HA	1.93	0.67
1:C:41:ASN:HB2	1:C:43:VAL:HG23	1.76	0.67
2:F:17:PRO:HB2	1:G:57:PRO:HG2	1.76	0.67
2:B:137:LEU:HB3	2:B:152:LYS:HD3	1.76	0.67
1:C:108:PHE:CE1	1:C:114:SER:HA	2.30	0.67
2:F:59:ASN:ND2	1:G:13:LYS:NZ	2.43	0.67
2:F:39:ASP:HB3	2:F:41:ASN:ND2	2.10	0.67
1:A:254:VAL:HG13	1:A:254:VAL:O	1.93	0.67
2:H:67:VAL:CG2	13:H:384:HOH:O	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:GLY:O	1:E:108:PHE:HD2	1.78	0.66
1:G:105:GLY:O	1:G:108:PHE:HD2	1.78	0.66
2:H:95:LEU:HD13	2:H:124:VAL:HG22	1.77	0.66
2:D:201:LEU:HG	2:D:205:LEU:CD2	2.26	0.66
9:E:288:ABU:HB1	2:H:208:TRP:HH2	1.60	0.66
1:E:111:LEU:HD12	13:E:436:HOH:O	1.94	0.66
10:H:289:GOL:H32	13:H:452:HOH:O	1.95	0.66
2:F:73:THR:O	2:F:170:LEU:HD12	1.94	0.66
1:G:135:VAL:CG1	13:G:371:HOH:O	2.43	0.66
2:B:172:THR:CG2	13:B:250:HOH:O	2.43	0.66
1:C:77:PHE:CE1	1:C:79:ILE:HD13	2.31	0.65
2:D:33:LEU:HG	2:D:35:LEU:CD1	2.26	0.65
13:E:270:HOH:O	2:F:190:LYS:HD3	1.94	0.65
2:F:35:LEU:O	2:F:50:GLY:HA3	1.94	0.65
1:E:22:GLN:NE2	1:E:102:PRO:HD3	2.11	0.65
1:C:249:LEU:HD22	1:C:253:LEU:CD2	2.27	0.65
2:H:67:VAL:HG23	13:H:384:HOH:O	1.94	0.65
1:C:49:LEU:O	1:C:49:LEU:HG	1.93	0.65
2:D:76:ARG:NH1	13:D:431:HOH:O	2.28	0.65
1:A:82:PRO:HD2	1:A:224:ILE:HG22	1.77	0.65
2:H:118:ASN:OD1	2:H:120:SER:HB2	1.97	0.65
1:A:108:PHE:HE1	1:A:114:SER:HA	1.62	0.65
1:A:253:LEU:O	1:A:255:ALA:N	2.30	0.65
2:F:59:ASN:H	9:F:290:ABU:HB1	1.62	0.65
2:F:10:SER:H	1:G:3:ASN:ND2	1.95	0.65
1:G:65:THR:OG1	1:G:67:VAL:HG22	1.95	0.64
1:C:67:VAL:CG1	1:C:239:SER:O	2.43	0.64
2:D:212:GLY:C	13:D:469:HOH:O	2.35	0.64
1:C:185:VAL:HG22	1:C:192:SER:HB3	1.80	0.64
1:A:170:LEU:HD22	1:A:253:LEU:HD21	1.79	0.64
1:E:16:GLN:HE21	1:E:18:ASN:HD21	1.46	0.64
2:H:35:LEU:O	2:H:50:GLY:HA3	1.97	0.64
2:B:51:ARG:HD2	2:B:102:PRO:HB3	1.79	0.64
1:E:254:VAL:O	1:E:256:ASN:N	2.29	0.64
2:F:112:PHE:HE1	13:F:257:HOH:O	1.81	0.64
2:H:1:THR:O	2:H:240:PHE:CD1	2.49	0.64
2:D:204:VAL:HG12	2:D:205:LEU:HD13	1.80	0.63
2:H:117:PHE:CZ	13:H:386:HOH:O	2.32	0.63
2:H:47:LYS:NZ	2:H:47:LYS:HB2	2.13	0.63
1:C:186:TYR:HB2	1:C:191:THR:HG22	1.80	0.63
1:E:181:VAL:HG11	10:E:279:GOL:H11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:THR:HG21	13:B:565:HOH:O	1.98	0.63
2:B:80:TYR:H	2:B:226:THR:HG22	1.64	0.63
2:H:21:LYS:HD3	13:H:280:HOH:O	1.98	0.63
1:A:59:ASN:HD21	2:D:13:LYS:HZ2	1.45	0.63
2:B:86:THR:CG2	2:B:86:THR:O	2.46	0.63
1:G:135:VAL:HG11	13:G:371:HOH:O	1.97	0.63
1:G:108:PHE:HE1	1:G:114:SER:HA	1.64	0.63
2:H:130:THR:HA	2:H:142:THR:HG22	1.80	0.63
1:A:253:LEU:C	1:A:255:ALA:N	2.52	0.63
9:E:288:ABU:HE2	2:H:59:ASN:HD22	1.64	0.62
2:F:108:PHE:HE1	2:F:114:SER:CA	2.13	0.62
2:B:39:ASP:HB2	2:B:40:LYS:HE2	1.81	0.62
2:D:84:ILE:HD11	2:D:161:LEU:HD23	1.81	0.62
1:E:253:LEU:CD2	2:F:170:LEU:HD21	2.29	0.62
2:D:79:ILE:HD11	2:D:91:LEU:HD22	1.82	0.62
1:E:84:ILE:HD13	1:E:163:ASN:HB2	1.82	0.62
2:F:158:LYS:HD3	13:F:273:HOH:O	1.99	0.61
1:E:211:ILE:HD13	1:E:212:GLY:N	2.14	0.61
2:B:3:ASN:ND2	1:C:10:SER:H	1.99	0.61
1:G:41:ASN:OD1	1:G:43:VAL:HG23	2.00	0.61
2:B:49:LEU:HD11	2:B:105:GLY:HA3	1.83	0.61
1:C:6:SER:HB3	1:C:235:ALA:HA	1.82	0.61
2:D:22:GLN:OE1	2:D:53:LEU:HD21	2.01	0.61
2:F:18:ASN:ND2	13:F:552:HOH:O	2.34	0.61
3:I:2:NAG:O3	3:I:3:BMA:C1	2.48	0.61
1:A:13:LYS:HZ2	2:D:59:ASN:HD21	1.48	0.60
2:D:67:VAL:HG23	2:D:238:LEU:HD21	1.83	0.60
9:B:276:ABU:HG2	13:B:589:HOH:O	2.00	0.60
2:B:40:LYS:N	2:B:40:LYS:CD	2.49	0.60
1:G:179:LEU:HD21	2:H:185:VAL:HG11	1.83	0.60
2:D:1:THR:O	2:D:240:PHE:HD2	1.85	0.60
2:F:137:LEU:HB2	2:F:152:LYS:HE2	1.82	0.60
1:A:13:LYS:NZ	2:D:240:PHE:HZ	2.00	0.60
1:E:67:VAL:HG13	1:E:238:LEU:HD11	1.84	0.60
1:E:185:VAL:HG22	1:E:192:SER:HB3	1.83	0.60
2:H:61:TRP:CE3	2:H:202:LYS:HG3	2.37	0.60
1:A:252:PHE:CD2	1:A:252:PHE:C	2.76	0.59
1:A:9:PHE:CZ	1:A:19:LEU:HD22	2.37	0.59
2:D:21:LYS:NZ	13:D:434:HOH:O	2.35	0.59
1:A:172:THR:CG2	13:A:275:HOH:O	2.41	0.59
1:E:47:LYS:HB3	1:E:47:LYS:HZ3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:186:TYR:HB2	2:H:191:THR:HG22	1.83	0.59
1:A:13:LYS:NZ	2:D:59:ASN:HD21	1.99	0.59
1:E:211:ILE:CD1	1:E:232:TRP:HZ2	2.15	0.59
1:G:8:THR:HB	1:G:233:SER:HB3	1.84	0.59
2:D:105:GLY:O	2:D:108:PHE:HD2	1.84	0.59
2:F:91:LEU:CD1	2:F:128:PHE:HB2	2.33	0.59
2:H:61:TRP:HA	13:H:261:HOH:O	2.01	0.59
1:A:108:PHE:HE1	1:A:114:SER:CA	2.16	0.59
2:D:188:SER:O	2:D:189:SER:CB	2.51	0.59
2:F:87:ILE:HD12	2:F:130:THR:HB	1.85	0.59
1:G:47:LYS:HZ2	1:G:47:LYS:HB3	1.65	0.59
2:H:78:THR:CG2	2:H:230:PHE:HZ	2.14	0.59
11:B:306:XYP:O2	4:J:3:BMA:O2	2.21	0.59
2:D:76:ARG:HH21	2:D:168:LYS:NZ	2.00	0.59
2:H:79:ILE:HG13	2:H:161:LEU:HD11	1.85	0.59
2:F:97:PRO:O	2:F:100:SER:N	2.36	0.59
1:C:230:PHE:CD1	13:C:494:HOH:O	2.48	0.59
9:E:288:ABU:HG2	2:H:3:ASN:HD22	1.64	0.59
1:A:127:GLU:OE1	1:A:147:ASP:OD2	2.20	0.58
1:E:252:PHE:O	1:E:256:ASN:CB	2.47	0.58
2:F:135:VAL:HG12	2:F:136:PHE:CE1	2.38	0.58
2:F:57:PRO:HG2	1:G:17:PRO:HB2	1.85	0.58
2:H:87:ILE:HD12	2:H:130:THR:CG2	2.33	0.58
1:A:185:VAL:HG11	2:B:179:LEU:HD21	1.84	0.58
2:F:139:PRO:HD2	2:F:143:HIS:CE1	2.39	0.58
1:A:108:PHE:CE1	1:A:114:SER:HA	2.38	0.58
1:C:108:PHE:HE1	1:C:114:SER:HA	1.68	0.58
1:A:134:THR:HA	13:A:299:HOH:O	2.02	0.58
2:H:230:PHE:HD1	13:H:257:HOH:O	1.86	0.57
2:B:80:TYR:H	2:B:226:THR:CG2	2.17	0.57
1:G:123:THR:H	1:G:149:ASN:ND2	2.01	0.57
1:A:130:THR:HG21	1:A:225:GLU:OE2	2.04	0.57
1:E:10:SER:HB3	2:H:1:THR:HG22	1.86	0.57
2:F:1:THR:O	2:F:240:PHE:HD2	1.87	0.57
2:D:87:ILE:HD12	2:D:130:THR:HB	1.86	0.57
1:A:12:PHE:HB2	1:A:31:GLY:O	2.04	0.57
1:G:254:VAL:O	2:H:237:LYS:HE2	2.05	0.57
2:H:122:GLN:N	2:H:149:ASN:ND2	2.53	0.57
2:B:157:VAL:HG21	13:B:252:HOH:O	2.05	0.57
1:A:157:VAL:HG22	1:A:158:LYS:H	1.70	0.57
1:E:5:ASP:OD2	9:E:284:ABU:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:LEU:HD12	13:G:290:HOH:O	2.02	0.57
1:A:179:LEU:HD13	1:A:181:VAL:HG23	1.85	0.56
1:G:36:THR:HG21	1:G:227:HIS:ND1	2.20	0.56
1:G:47:LYS:CB	1:G:47:LYS:NZ	2.64	0.56
1:A:133:ASN:O	1:A:138:ASP:HB2	2.05	0.56
1:A:254:VAL:O	1:A:255:ALA:CB	2.42	0.56
2:F:22:GLN:NE2	2:F:51:ARG:HE	2.02	0.56
2:F:69:ALA:HB2	2:F:238:LEU:HB2	1.87	0.56
2:B:173:TYR:CE2	2:B:201:LEU:HD22	2.41	0.56
10:C:283:GOL:H31	2:D:181:VAL:HG11	1.87	0.56
1:E:249:LEU:O	1:E:250:ALA:C	2.43	0.56
1:G:142:THR:HG23	13:G:259:HOH:O	2.03	0.56
2:B:1:THR:O	2:B:240:PHE:HD1	1.88	0.56
2:B:59:ASN:N	9:B:276:ABU:HB2	2.17	0.56
2:B:240:PHE:HE2	1:C:13:LYS:HZ1	1.52	0.56
1:E:157:VAL:CG2	1:E:195:LEU:HB2	2.34	0.56
2:H:105:GLY:O	2:H:108:PHE:CD2	2.52	0.56
1:A:13:LYS:HZ2	2:D:59:ASN:ND2	2.03	0.56
1:E:254:VAL:C	1:E:256:ASN:N	2.59	0.56
2:F:22:GLN:HE22	2:F:51:ARG:HE	1.52	0.56
1:G:78:THR:HG1	1:G:230:PHE:HZ	1.45	0.56
2:H:65:THR:OG1	2:H:67:VAL:HG12	2.06	0.56
2:F:65:THR:OG1	2:F:67:VAL:CG1	2.51	0.56
1:A:67:VAL:HG12	1:A:238:LEU:CD1	2.36	0.56
1:C:122:GLN:HB3	1:C:206:PRO:HD3	1.87	0.56
1:A:59:ASN:HD21	2:D:13:LYS:NZ	2.03	0.56
1:G:178:LYS:O	1:G:198:VAL:HA	2.06	0.56
1:G:79:ILE:HD12	1:G:225:GLU:HB2	1.88	0.55
1:E:59:ASN:HD21	2:H:13:LYS:HZ2	1.53	0.55
1:A:237:LYS:HZ3	1:A:247:LEU:N	2.04	0.55
2:B:79:ILE:HB	2:B:226:THR:O	2.05	0.55
1:E:194:ILE:HG23	2:F:192:SER:HB3	1.89	0.55
2:B:86:THR:HG22	2:B:222:GLY:O	2.05	0.55
1:E:115:ALA:CB	13:E:271:HOH:O	2.54	0.55
1:E:57:PRO:HA	1:E:209:VAL:O	2.06	0.55
1:C:5:ASP:OD2	9:C:282:ABU:N	2.40	0.55
1:E:59:ASN:HD21	2:H:13:LYS:NZ	2.05	0.55
1:C:157:VAL:CG2	13:C:321:HOH:O	2.29	0.55
2:H:79:ILE:HD13	2:H:225:GLU:CG	2.37	0.55
11:B:306:XYP:C1	4:J:3:BMA:HO2	2.12	0.55
1:C:77:PHE:HE1	1:C:79:ILE:HD13	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LYS:NZ	2:D:240:PHE:CZ	2.74	0.55
2:H:79:ILE:O	2:H:79:ILE:HG13	2.07	0.55
1:A:165:GLU:CG	1:A:188:SER:OG	2.55	0.55
1:C:7:PHE:CE1	1:C:9:PHE:CE2	2.95	0.55
2:F:91:LEU:HD13	2:F:128:PHE:HB2	1.88	0.55
1:A:137:LEU:HG	1:A:152:LYS:HE2	1.89	0.55
2:H:132:GLU:HG3	2:H:140:PRO:HA	1.89	0.55
2:B:77:PHE:CE1	2:B:91:LEU:HD21	2.42	0.54
2:D:22:GLN:HB2	2:D:51:ARG:HB2	1.88	0.54
2:F:36:THR:OG1	2:F:227:HIS:HD2	1.90	0.54
2:B:35:LEU:O	2:B:50:GLY:HA3	2.08	0.54
1:C:44:PRO:O	1:C:224:ILE:HD12	2.06	0.54
2:B:206:PRO:HD2	2:B:209:VAL:CG1	2.37	0.54
1:E:18:ASN:OD1	9:E:288:ABU:N	2.41	0.54
2:F:59:ASN:H	9:F:290:ABU:CB	2.19	0.54
2:H:158:LYS:HE3	2:H:160:ASP:OD1	2.07	0.54
2:H:225:GLU:OE2	2:H:227:HIS:CE1	2.59	0.54
1:A:1:THR:O	1:A:240:PHE:CD2	2.57	0.54
2:B:86:THR:CG2	2:B:222:GLY:O	2.56	0.54
9:E:288:ABU:HG2	2:H:3:ASN:HD21	1.64	0.54
2:B:240:PHE:HE2	1:C:13:LYS:NZ	2.05	0.54
2:D:36:THR:HG21	2:D:217:THR:CG2	2.35	0.54
1:A:144:ILE:HG22	1:A:195:LEU:HD23	1.90	0.54
1:E:170:LEU:HD22	1:E:253:LEU:HD11	1.89	0.54
2:H:201:LEU:HG	2:H:205:LEU:CD2	2.38	0.54
10:H:289:GOL:C2	13:H:411:HOH:O	2.26	0.54
2:B:118:ASN:O	2:B:149:ASN:HB3	2.07	0.54
2:D:76:ARG:HH21	2:D:168:LYS:HZ1	1.56	0.54
1:E:211:ILE:HD13	1:E:211:ILE:C	2.28	0.54
1:C:135:VAL:HG12	13:C:305:HOH:O	2.07	0.53
1:A:49:LEU:CD1	1:A:105:GLY:CA	2.85	0.53
1:A:57:PRO:HG2	2:D:17:PRO:HB2	1.91	0.53
1:C:1:THR:O	1:C:240:PHE:HD1	1.91	0.53
1:G:68:VAL:HG22	1:G:175:SER:CB	2.37	0.53
2:H:86:THR:HG22	2:H:223:TYR:HA	1.89	0.53
2:H:122:GLN:N	2:H:149:ASN:HD21	2.07	0.53
1:A:79:ILE:HD13	1:A:225:GLU:CB	2.37	0.53
1:C:127:GLU:OE1	1:C:147:ASP:OD2	2.27	0.53
2:F:41:ASN:ND2	2:F:43:VAL:HG13	2.23	0.53
1:A:79:ILE:HG13	1:A:161:LEU:HD11	1.91	0.53
1:E:13:LYS:NZ	2:H:59:ASN:HD21	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:78:THR:HG22	2:H:230:PHE:CZ	2.44	0.53
1:E:249:LEU:O	1:E:252:PHE:HB3	2.09	0.53
2:F:135:VAL:HG12	2:F:136:PHE:CD1	2.43	0.53
2:F:201:LEU:HG	2:F:205:LEU:HD12	1.91	0.53
1:E:79:ILE:HG13	1:E:161:LEU:HD11	1.90	0.52
1:E:67:VAL:CG2	1:E:239:SER:O	2.49	0.52
2:F:121:TYR:O	2:F:123:THR:HG23	2.09	0.52
1:E:173:TYR:CE2	1:E:201:LEU:HD22	2.44	0.52
1:E:97:PRO:HD3	1:E:122:GLN:O	2.08	0.52
1:A:99:SER:HB3	13:A:575:HOH:O	2.09	0.52
2:B:97:PRO:O	2:B:100:SER:HB2	2.10	0.52
2:D:84:ILE:HD13	2:D:163:ASN:HB2	1.91	0.52
2:F:58:ILE:HG23	9:F:290:ABU:HE2	1.91	0.52
1:E:1:THR:O	1:E:1:THR:HG22	2.10	0.52
2:F:35:LEU:HD21	2:F:213:PHE:HB3	1.92	0.52
2:H:27:VAL:HG12	2:H:28:THR:O	2.09	0.52
2:B:22:GLN:OE1	2:B:51:ARG:HD3	2.08	0.52
2:B:5:ASP:C	2:B:6:SER:OG	2.47	0.52
2:H:67:VAL:HG23	13:H:258:HOH:O	2.09	0.52
1:A:172:THR:HG22	1:A:181:VAL:HB	1.91	0.52
2:B:147:ASP:HB3	2:B:150:SER:O	2.10	0.52
1:A:247:LEU:HD13	1:A:248:ASP:H	1.74	0.52
1:A:82:PRO:HD2	1:A:224:ILE:CG2	2.40	0.52
1:C:78:THR:HG1	1:C:230:PHE:HE2	1.54	0.52
1:G:60:ILE:HG21	1:G:205:LEU:HD23	1.91	0.52
1:G:2:THR:HB	1:G:239:SER:HA	1.91	0.52
1:C:226:THR:HA	13:C:277:HOH:O	2.08	0.52
1:A:103:LYS:O	1:A:110:GLY:HA2	2.10	0.52
2:B:127:GLU:OE1	2:B:147:ASP:OD2	2.28	0.52
2:B:49:LEU:HD13	13:B:278:HOH:O	2.10	0.52
1:E:93:PHE:CE1	1:E:211:ILE:CD1	2.80	0.52
2:F:123:THR:H	2:F:149:ASN:ND2	2.08	0.52
1:G:196:SER:HB2	13:G:290:HOH:O	2.09	0.52
1:A:59:ASN:N	9:A:280:ABU:HE2	2.19	0.51
1:A:135:VAL:HG22	13:A:362:HOH:O	2.09	0.51
1:A:254:VAL:HG12	1:A:254:VAL:O	2.09	0.51
1:C:185:VAL:CG1	2:D:179:LEU:HD21	2.36	0.51
1:E:44:PRO:HG2	1:E:224:ILE:CG2	2.30	0.51
1:G:117:PHE:C	1:G:117:PHE:CD2	2.84	0.51
1:C:21:LYS:NZ	1:C:33:LEU:HD13	2.25	0.51
2:H:133:ASN:HB3	2:H:135:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:LEU:CD2	1:C:253:LEU:CD2	2.89	0.51
2:D:179:LEU:HD12	2:D:197:ASP:O	2.10	0.51
1:G:200:ASP:OD1	1:G:202:LYS:HE2	2.11	0.51
1:E:201:LEU:HG	1:E:205:LEU:CD1	2.38	0.51
2:H:117:PHE:CD2	2:H:118:ASN:N	2.78	0.51
1:G:79:ILE:HD13	1:G:225:GLU:CG	2.41	0.51
2:H:47:LYS:HZ3	2:H:47:LYS:HB2	1.74	0.51
1:A:157:VAL:HG22	1:A:158:LYS:N	2.26	0.51
2:D:157:VAL:HG12	2:D:195:LEU:HB2	1.93	0.51
1:G:157:VAL:HG22	13:G:272:HOH:O	2.11	0.51
1:C:58:ILE:HA	9:C:282:ABU:CA	2.41	0.50
2:F:56:SER:CB	13:G:547:HOH:O	2.40	0.50
1:G:108:PHE:CE1	1:G:114:SER:HA	2.44	0.50
2:H:238:LEU:C	2:H:238:LEU:CD2	2.80	0.50
2:H:87:ILE:CG1	2:H:130:THR:HG22	2.40	0.50
1:A:165:GLU:HG2	1:A:188:SER:OG	2.10	0.50
1:E:73:THR:HG21	1:E:93:PHE:CZ	2.46	0.50
1:G:73:THR:HB	1:G:234:PHE:HD1	1.76	0.50
2:B:36:THR:OG1	2:B:227:HIS:CD2	2.56	0.50
2:H:108:PHE:HE1	2:H:114:SER:HA	1.76	0.50
2:H:191:THR:HG23	2:H:193:PHE:CE2	2.47	0.50
1:C:237:LYS:HB3	1:C:247:LEU:HD13	1.93	0.50
1:A:17:PRO:HB2	2:D:57:PRO:HG2	1.92	0.50
1:E:22:GLN:HE22	1:E:102:PRO:HD3	1.73	0.50
2:B:62:ASP:O	2:B:66:GLY:N	2.44	0.50
2:B:65:THR:OG1	2:B:67:VAL:HG12	2.11	0.50
2:B:76:ARG:CB	13:B:429:HOH:O	2.59	0.50
1:G:117:PHE:CD2	1:G:118:ASN:N	2.80	0.50
1:A:201:LEU:HG	1:A:205:LEU:HD12	1.94	0.49
2:F:142:THR:CG2	2:F:159:TRP:CE3	2.95	0.49
1:A:170:LEU:CD2	1:A:253:LEU:HD21	2.42	0.49
1:A:36:THR:CG2	1:A:227:HIS:CD2	2.76	0.49
1:C:36:THR:OG1	1:C:227:HIS:HD2	1.95	0.49
1:G:179:LEU:HD21	2:H:185:VAL:CG1	2.41	0.49
2:H:122:GLN:H	2:H:149:ASN:ND2	2.10	0.49
2:H:68:VAL:HB	2:H:175:SER:OG	2.12	0.49
1:A:194:ILE:HD13	2:B:192:SER:HB3	1.93	0.49
2:B:5:ASP:OD2	9:B:276:ABU:N	2.45	0.49
2:D:49:LEU:HD12	2:D:105:GLY:CA	2.42	0.49
1:E:115:ALA:HB3	13:E:271:HOH:O	2.11	0.49
1:G:181:VAL:HG22	1:G:196:SER:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:TRP:CD2	2:H:202:LYS:HG3	2.48	0.49
1:C:124:VAL:HG21	1:C:201:LEU:CD2	2.42	0.49
2:H:11:LYS:O	13:H:432:HOH:O	2.20	0.49
2:H:137:LEU:HB3	3:I:1:NAG:H83	1.95	0.49
1:A:67:VAL:HG12	1:A:238:LEU:HD11	1.95	0.49
2:B:144:ILE:HG13	2:B:159:TRP:HB2	1.93	0.49
1:G:247:LEU:O	1:G:248:ASP:HB3	2.12	0.49
2:H:136:PHE:O	2:H:152:LYS:HG2	2.12	0.49
2:H:238:LEU:C	2:H:238:LEU:HD22	2.33	0.49
1:A:194:ILE:HG13	2:B:194:ILE:HB	1.95	0.49
2:D:16:GLN:HG2	2:D:18:ASN:OD1	2.13	0.49
1:E:69:ALA:O	1:E:175:SER:HB3	2.12	0.49
2:H:101:PRO:O	2:H:103:LYS:NZ	2.40	0.49
2:H:186:TYR:HD2	2:H:191:THR:CG2	2.26	0.49
4:J:3:BMA:O4	4:J:4:MAN:C1	2.60	0.49
1:C:41:ASN:HA	13:C:467:HOH:O	2.12	0.49
2:D:1:THR:HB	2:D:240:PHE:HB2	1.94	0.49
2:B:59:ASN:HB3	13:B:589:HOH:O	2.12	0.48
2:D:60:ILE:HD11	2:D:206:PRO:O	2.13	0.48
2:D:76:ARG:HA	2:D:167:ALA:O	2.14	0.48
2:H:115:ALA:O	2:H:152:LYS:HD2	2.14	0.48
2:D:172:THR:O	2:D:180:LEU:HD12	2.12	0.48
2:D:185:VAL:O	2:D:187:PRO:HD3	2.12	0.48
2:D:52:ALA:O	2:D:212:GLY:HA3	2.13	0.48
2:F:74:SER:HA	2:F:169:VAL:O	2.14	0.48
1:G:153:SER:HB3	1:G:155:LYS:O	2.13	0.48
1:G:87:ILE:HB	1:G:225:GLU:OE1	2.13	0.48
2:B:206:PRO:HD2	2:B:209:VAL:HG12	1.95	0.48
1:C:79:ILE:HG23	1:C:225:GLU:HG3	1.96	0.48
2:F:78:THR:HG1	2:F:230:PHE:HE2	1.55	0.48
2:H:33:LEU:HD23	2:H:229:VAL:HB	1.95	0.48
2:H:137:LEU:HB3	3:I:1:NAG:C8	2.43	0.48
1:A:58:ILE:HG23	9:A:280:ABU:HG2	1.96	0.48
1:G:130:THR:HA	1:G:142:THR:HG22	1.96	0.48
2:B:157:VAL:HG22	13:B:286:HOH:O	2.13	0.48
1:E:76:ARG:HA	1:E:167:ALA:O	2.14	0.48
2:H:27:VAL:HG23	13:H:280:HOH:O	2.13	0.48
1:E:4:THR:HG22	1:E:237:LYS:HB3	1.96	0.48
2:F:121:TYR:O	2:F:123:THR:CG2	2.62	0.48
2:F:76:ARG:HA	2:F:167:ALA:O	2.13	0.48
2:B:76:ARG:HG2	2:B:230:PHE:HD2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:ARG:HB2	13:B:429:HOH:O	2.13	0.48
1:G:205:LEU:HG	1:G:209:VAL:HG21	1.96	0.48
1:A:157:VAL:CG2	13:A:259:HOH:O	2.53	0.48
1:A:130:THR:HG21	1:A:225:GLU:CD	2.34	0.48
1:A:225:GLU:OE2	1:A:227:HIS:HE1	1.97	0.48
2:F:1:THR:O	2:F:240:PHE:CD2	2.67	0.48
1:G:12:PHE:O	1:G:31:GLY:HA2	2.13	0.48
2:F:13:LYS:HZ3	1:G:240:PHE:HE1	1.60	0.48
1:A:86:THR:O	1:A:223:TYR:HA	2.14	0.47
1:C:7:PHE:CE1	1:C:9:PHE:HE2	2.32	0.47
1:G:75:PHE:CZ	1:G:169:VAL:HG11	2.48	0.47
2:H:121:TYR:HB2	2:H:149:ASN:HD22	1.78	0.47
2:B:207:GLU:CG	13:B:256:HOH:O	2.51	0.47
2:F:77:PHE:HA	2:F:228:ASP:O	2.14	0.47
11:B:306:XYP:C1	4:J:3:BMA:H2	2.44	0.47
1:C:1:THR:O	1:C:240:PHE:CD1	2.66	0.47
1:E:142:THR:HG22	1:E:159:TRP:CE3	2.49	0.47
1:C:151:ILE:HG22	13:C:258:HOH:O	2.12	0.47
1:G:21:LYS:HB2	1:G:21:LYS:NZ	2.28	0.47
2:B:47:LYS:HE3	2:B:219:ALA:HA	1.96	0.47
2:F:33:LEU:HG	2:F:35:LEU:HD13	1.97	0.47
1:G:49:LEU:HD13	1:G:49:LEU:HA	1.70	0.47
2:B:47:LYS:HA	2:B:47:LYS:HD3	1.60	0.47
1:C:116:VAL:HG22	13:C:265:HOH:O	2.14	0.47
2:F:98:VAL:HG13	2:F:98:VAL:O	2.15	0.47
1:A:179:LEU:HD13	1:A:181:VAL:CG2	2.44	0.47
1:E:105:GLY:O	1:E:108:PHE:CD2	2.63	0.47
1:A:96:ALA:HB1	1:A:97:PRO:HD2	1.96	0.47
2:F:240:PHE:HE1	1:G:13:LYS:HZ1	1.61	0.47
1:G:117:PHE:HZ	13:G:438:HOH:O	1.97	0.47
1:G:78:THR:HG1	1:G:230:PHE:HE2	1.53	0.47
1:A:58:ILE:HA	9:A:280:ABU:CA	2.45	0.47
2:B:21:LYS:HB3	2:B:21:LYS:NZ	2.26	0.47
2:B:79:ILE:O	2:B:79:ILE:HG13	2.15	0.47
2:F:33:LEU:HD23	2:F:229:VAL:HB	1.96	0.47
2:B:225:GLU:OE2	2:B:227:HIS:HE1	1.97	0.47
1:C:21:LYS:HD3	1:C:21:LYS:HA	1.61	0.47
1:E:67:VAL:HG11	1:E:240:PHE:HA	1.96	0.47
1:C:206:PRO:HD2	1:C:209:VAL:HG12	1.97	0.47
1:E:46:PRO:HB3	1:E:224:ILE:HD11	1.97	0.46
1:E:1:THR:O	1:E:240:PHE:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4:THR:OG1	1:G:8:THR:HG23	2.14	0.46
2:B:5:ASP:HB2	9:B:276:ABU:HE2	1.97	0.46
2:D:12:PHE:HB2	2:D:31:GLY:O	2.14	0.46
1:E:52:ALA:C	1:E:53:LEU:HD12	2.36	0.46
2:F:225:GLU:OE2	2:F:227:HIS:HE1	1.99	0.46
1:A:123:THR:H	1:A:149:ASN:ND2	2.13	0.46
1:C:124:VAL:HG21	1:C:201:LEU:HD23	1.98	0.46
1:G:37:LYS:HE3	13:G:282:HOH:O	2.15	0.46
1:C:47:LYS:HB3	1:C:47:LYS:HE3	1.54	0.46
9:E:288:ABU:CD	2:H:3:ASN:HD21	2.29	0.46
1:G:197:ASP:N	13:G:290:HOH:O	2.48	0.46
1:A:67:VAL:HG11	1:A:239:SER:C	2.28	0.46
2:F:41:ASN:HD22	2:F:42:GLY:N	2.13	0.46
1:G:167:ALA:HB2	1:G:186:TYR:CE1	2.51	0.46
2:H:78:THR:HG22	2:H:228:ASP:HB2	1.96	0.46
2:B:21:LYS:HZ2	2:B:21:LYS:CB	2.28	0.46
2:B:58:ILE:HG23	9:B:276:ABU:HB1	1.98	0.46
1:A:247:LEU:HD13	1:A:248:ASP:N	2.30	0.46
2:B:123:THR:H	2:B:149:ASN:ND2	2.14	0.46
1:C:190:LYS:HD2	2:D:197:ASP:OD1	2.16	0.46
2:F:98:VAL:HA	2:F:99:SER:HA	1.62	0.46
1:A:225:GLU:OE2	1:A:227:HIS:CE1	2.69	0.46
1:A:1:THR:HG21	2:D:11:LYS:HG3	1.97	0.46
2:B:22:GLN:HB2	2:B:51:ARG:HB2	1.98	0.46
2:H:79:ILE:HD13	2:H:225:GLU:HG3	1.98	0.46
1:A:79:ILE:HD13	1:A:225:GLU:CG	2.46	0.45
2:F:225:GLU:OE2	2:F:227:HIS:CE1	2.69	0.45
1:G:178:LYS:HB2	1:G:198:VAL:HG13	1.97	0.45
1:C:39:ASP:C	1:C:39:ASP:OD2	2.54	0.45
9:F:290:ABU:N	1:G:18:ASN:ND2	2.58	0.45
13:B:422:HOH:O	1:G:133:ASN:HA	2.15	0.45
2:H:78:THR:HG22	2:H:230:PHE:HZ	1.79	0.45
2:H:78:THR:CG2	2:H:230:PHE:CZ	2.98	0.45
1:A:224:ILE:O	1:A:224:ILE:HG22	2.16	0.45
2:B:226:THR:HA	13:B:287:HOH:O	2.16	0.45
2:F:144:ILE:HD12	2:F:159:TRP:HB2	1.98	0.45
4:J:3:BMA:O4	4:J:4:MAN:C2	2.64	0.45
1:G:79:ILE:CD1	1:G:225:GLU:CB	2.88	0.45
1:A:83:ASN:HD22	1:A:85:ALA:H	1.65	0.45
1:C:12:PHE:HB2	1:C:31:GLY:O	2.17	0.45
1:C:56:SER:HA	1:C:57:PRO:HD3	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:ILE:HD13	1:E:225:GLU:CD	2.37	0.45
1:G:201:LEU:HG	1:G:205:LEU:CD2	2.39	0.45
2:H:67:VAL:HG13	2:H:238:LEU:CD2	2.43	0.45
2:B:133:ASN:O	2:B:138:ASP:HB2	2.17	0.45
2:B:89:ASP:OD2	2:B:218:GLY:HA2	2.16	0.45
1:C:78:THR:OG1	1:C:230:PHE:HE2	1.99	0.45
1:A:233:SER:OG	1:A:256:ASN:HB3	2.16	0.45
1:A:67:VAL:HG12	1:A:238:LEU:HD12	1.98	0.45
1:A:61:TRP:CE3	1:A:202:LYS:HG3	2.52	0.45
2:B:207:GLU:CD	13:B:256:HOH:O	2.55	0.45
1:E:79:ILE:HB	1:E:226:THR:O	2.17	0.45
1:A:73:THR:HA	1:A:233:SER:O	2.16	0.45
1:A:77:PHE:HE1	1:A:79:ILE:CG2	2.30	0.45
2:D:77:PHE:HE1	2:D:79:ILE:HG12	1.82	0.45
1:E:235:ALA:HB1	1:E:247:LEU:HD13	1.98	0.45
2:H:137:LEU:HG	2:H:152:LYS:HE2	1.98	0.45
1:A:117:PHE:HZ	13:A:272:HOH:O	1.99	0.45
1:E:17:PRO:HB2	2:H:57:PRO:HG2	1.99	0.45
1:G:78:THR:CB	1:G:230:PHE:HZ	2.30	0.45
2:H:213:PHE:HE2	2:H:232:TRP:CD2	2.35	0.45
2:F:9:PHE:CE1	2:F:18:ASN:ND2	2.71	0.45
2:H:108:PHE:HB3	2:H:112:PHE:O	2.17	0.45
1:C:122:GLN:H	1:C:149:ASN:ND2	2.14	0.44
1:G:173:TYR:CE2	1:G:201:LEU:HD22	2.52	0.44
1:G:183:ALA:HA	1:G:193:PHE:O	2.17	0.44
1:A:196:SER:CB	2:B:192:SER:HG	2.29	0.44
2:B:81:ALA:HB1	2:B:87:ILE:HG22	1.99	0.44
1:C:77:PHE:CD1	1:C:79:ILE:HD13	2.53	0.44
2:D:103:LYS:HB3	2:D:113:ASP:OD1	2.17	0.44
1:E:12:PHE:O	1:E:31:GLY:HA2	2.18	0.44
1:E:225:GLU:OE2	1:E:227:HIS:HE1	2.00	0.44
1:E:24:ASP:HB2	1:E:49:LEU:O	2.16	0.44
2:H:144:ILE:HG13	2:H:159:TRP:HB2	1.98	0.44
1:E:18:ASN:HD22	1:E:18:ASN:C	2.20	0.44
2:D:188:SER:N	13:D:461:HOH:O	2.48	0.44
2:F:103:LYS:HG2	2:F:113:ASP:OD1	2.17	0.44
1:E:68:VAL:HB	1:E:175:SER:HB2	1.99	0.44
1:C:135:VAL:CG1	13:C:305:HOH:O	2.64	0.44
1:C:122:GLN:H	1:C:149:ASN:HD21	1.66	0.44
2:B:21:LYS:HZ2	2:B:21:LYS:HB3	1.83	0.44
2:F:49:LEU:CD2	2:F:105:GLY:CA	2.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:118:ASN:OD1	2:F:120:SER:HB2	2.18	0.44
2:F:41:ASN:C	2:F:41:ASN:HD22	2.21	0.44
1:G:122:GLN:HB3	1:G:206:PRO:HD3	1.98	0.44
2:H:200:ASP:O	2:H:203:SER:HB2	2.17	0.44
2:B:20:LYS:HE3	2:B:22:GLN:HE21	1.82	0.44
1:E:194:ILE:CG2	2:F:192:SER:HB3	2.48	0.44
2:F:59:ASN:HD22	1:G:13:LYS:HZ2	1.59	0.44
1:A:124:VAL:CB	13:A:297:HOH:O	2.63	0.43
2:B:79:ILE:HD12	2:B:225:GLU:HB2	2.00	0.43
1:C:88:ALA:HA	1:C:89:ASP:HA	1.77	0.43
2:D:59:ASN:HD22	9:D:278:ABU:CD	2.31	0.43
1:E:211:ILE:HD12	1:E:232:TRP:HZ2	1.80	0.43
1:G:79:ILE:HD13	1:G:225:GLU:HB2	1.96	0.43
1:G:35:LEU:O	1:G:50:GLY:HA3	2.18	0.43
1:G:222:GLY:O	1:G:224:ILE:HG12	2.18	0.43
1:A:13:LYS:CE	2:D:240:PHE:CZ	3.01	0.43
1:C:77:PHE:CD1	1:C:79:ILE:CD1	3.02	0.43
1:E:100:SER:HB2	13:E:267:HOH:O	2.17	0.43
1:C:60:ILE:HD13	1:C:60:ILE:HA	1.84	0.43
2:D:147:ASP:HB3	2:D:150:SER:O	2.18	0.43
2:F:62:ASP:HB3	2:F:67:VAL:CG1	2.49	0.43
1:G:252:PHE:CD1	1:G:256:ASN:HB2	2.53	0.43
1:G:252:PHE:O	1:G:256:ASN:N	2.36	0.43
1:E:35:LEU:O	1:E:50:GLY:HA3	2.18	0.43
1:C:240:PHE:N	1:C:240:PHE:CD1	2.86	0.43
1:G:138:ASP:HB3	1:G:143:HIS:CE1	2.53	0.43
1:A:7:PHE:C	1:A:7:PHE:CD1	2.92	0.43
1:E:61:TRP:CE3	1:E:202:LYS:HG3	2.52	0.43
1:E:65:THR:HB	1:E:67:VAL:HG12	2.00	0.43
2:F:213:PHE:HE2	2:F:232:TRP:CD2	2.36	0.43
2:B:41:ASN:O	1:G:135:VAL:HB	2.19	0.43
1:G:122:GLN:N	1:G:149:ASN:HD21	2.17	0.43
2:D:43:VAL:HA	2:D:44:PRO:HD2	1.75	0.43
1:E:114:SER:OG	1:E:116:VAL:CG2	2.66	0.43
2:H:79:ILE:CD1	2:H:225:GLU:HB2	2.48	0.43
1:A:84:ILE:HD12	1:A:87:ILE:HG21	2.01	0.43
2:B:201:LEU:HG	2:B:205:LEU:CD1	2.47	0.43
2:B:69:ALA:O	2:B:175:SER:HB3	2.18	0.43
1:A:254:VAL:HG23	2:B:72:ALA:CB	2.48	0.43
2:D:79:ILE:HG23	2:D:225:GLU:HG3	2.01	0.43
1:A:19:LEU:HD12	1:A:21:LYS:NZ	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:GLY:O	1:C:108:PHE:HD2	2.00	0.43
1:C:185:VAL:HG11	2:D:179:LEU:CD2	2.40	0.43
1:E:22:GLN:NE2	1:E:102:PRO:HG3	2.34	0.43
1:E:170:LEU:HD22	1:E:253:LEU:CD1	2.48	0.43
1:E:22:GLN:HE21	1:E:102:PRO:HG3	1.82	0.43
2:F:37:LYS:HE2	13:F:255:HOH:O	2.18	0.43
2:F:88:ALA:HA	2:F:89:ASP:HA	1.67	0.43
1:G:1:THR:O	1:G:240:PHE:HD2	2.02	0.43
1:A:35:LEU:O	1:A:50:GLY:HA3	2.19	0.42
1:A:58:ILE:HG23	9:A:280:ABU:CG	2.49	0.42
2:B:158:LYS:N	13:B:282:HOH:O	2.46	0.42
2:D:14:PRO:HA	2:D:27:VAL:HG13	2.01	0.42
2:F:49:LEU:CD2	2:F:105:GLY:HA2	2.27	0.42
2:H:87:ILE:CD1	2:H:130:THR:CG2	2.97	0.42
2:H:79:ILE:HB	2:H:226:THR:O	2.19	0.42
1:A:249:LEU:HD21	2:B:170:LEU:HD22	2.01	0.42
1:C:103:LYS:HB3	1:C:113:ASP:OD1	2.20	0.42
1:E:201:LEU:HA	1:E:201:LEU:HD12	1.84	0.42
2:F:91:LEU:HB3	2:F:215:ALA:HB2	2.01	0.42
1:G:74:SER:HA	1:G:169:VAL:O	2.20	0.42
1:A:144:ILE:HG22	1:A:195:LEU:CD2	2.49	0.42
1:C:84:ILE:HG12	1:C:163:ASN:HD22	1.84	0.42
2:F:57:PRO:HG3	2:F:98:VAL:HG21	2.00	0.42
1:G:21:LYS:HD3	1:G:21:LYS:HA	1.84	0.42
3:L:2:NAG:O5	3:L:4:FUC:H5	2.19	0.42
1:A:41:ASN:HB3	1:A:43:VAL:HG23	2.02	0.42
2:D:188:SER:O	2:D:188:SER:OG	2.37	0.42
2:D:230:PHE:CD2	13:D:244:HOH:O	2.43	0.42
1:E:4:THR:HA	1:E:236:SER:O	2.19	0.42
1:G:96:ALA:HB1	1:G:97:PRO:HD2	2.00	0.42
2:B:38:VAL:HA	2:B:44:PRO:HA	2.01	0.42
2:B:5:ASP:C	2:B:6:SER:HG	2.23	0.42
2:B:13:LYS:HE2	1:C:240:PHE:CE2	2.54	0.42
1:A:117:PHE:HA	1:A:150:SER:HB2	2.01	0.42
2:F:147:ASP:OD1	2:F:153:SER:OG	2.20	0.42
2:F:76:ARG:HG3	2:F:230:PHE:HB2	2.00	0.42
1:G:21:LYS:CB	1:G:21:LYS:NZ	2.83	0.42
1:G:58:ILE:HG23	9:G:286:ABU:HE2	2.00	0.42
2:H:51:ARG:HG3	2:H:214:SER:OG	2.19	0.42
2:B:59:ASN:HB2	2:B:208:TRP:CH2	2.55	0.42
2:B:240:PHE:CE2	1:C:13:LYS:NZ	2.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:LYS:HE3	2:D:25:ALA:O	2.20	0.42
1:E:252:PHE:O	1:E:256:ASN:N	2.52	0.42
1:G:36:THR:HG21	1:G:217:THR:HG23	2.02	0.42
2:H:167:ALA:HB2	2:H:186:TYR:CE1	2.55	0.42
2:H:49:LEU:HD22	2:H:50:GLY:N	2.34	0.42
1:A:74:SER:HA	1:A:169:VAL:O	2.20	0.42
1:C:200:ASP:O	1:C:201:LEU:CB	2.58	0.42
1:C:21:LYS:HZ2	1:C:33:LEU:HD13	1.84	0.42
1:C:36:THR:O	1:C:38:VAL:HG23	2.20	0.42
1:E:117:PHE:C	1:E:117:PHE:CD2	2.92	0.42
2:H:137:LEU:CD2	2:H:152:LYS:HE2	2.50	0.42
9:E:288:ABU:HE2	2:H:59:ASN:ND2	2.31	0.42
1:G:47:LYS:HZ2	1:G:47:LYS:CB	2.29	0.42
2:H:91:LEU:HD23	2:H:128:PHE:HB2	2.02	0.42
1:E:181:VAL:HG21	10:E:279:GOL:O2	2.19	0.41
1:A:100:SER:HB3	13:A:472:HOH:O	2.20	0.41
2:B:116:VAL:HG21	4:J:1:NAG:H81	2.01	0.41
2:B:157:VAL:HG22	2:B:158:LYS:H	1.85	0.41
2:D:93:PHE:HD1	13:D:469:HOH:O	2.03	0.41
1:E:96:ALA:HB1	1:E:97:PRO:CD	2.50	0.41
2:F:97:PRO:HD3	2:F:122:GLN:O	2.20	0.41
1:G:78:THR:HB	1:G:230:PHE:HZ	1.84	0.41
2:B:21:LYS:HE3	2:B:21:LYS:HB3	1.64	0.41
9:F:290:ABU:HB2	13:F:590:HOH:O	2.19	0.41
1:G:8:THR:HB	1:G:233:SER:CB	2.50	0.41
1:A:33:LEU:HD22	1:A:35:LEU:HD13	2.02	0.41
2:B:97:PRO:O	2:B:100:SER:CB	2.69	0.41
1:C:249:LEU:HD22	1:C:253:LEU:HD23	1.99	0.41
1:A:40:LYS:C	1:A:42:GLY:H	2.24	0.41
2:B:87:ILE:HB	2:B:225:GLU:OE1	2.20	0.41
1:C:65:THR:HG23	1:C:67:VAL:HG23	2.02	0.41
2:D:49:LEU:HD12	2:D:105:GLY:HA2	2.01	0.41
1:G:86:THR:HG23	1:G:223:TYR:CE2	2.55	0.41
1:G:249:LEU:O	1:G:250:ALA:C	2.58	0.41
1:A:118:ASN:HB3	1:A:121:TYR:CD2	2.56	0.41
1:A:252:PHE:CD2	1:A:253:LEU:N	2.89	0.41
1:C:73:THR:HB	1:C:234:PHE:HD1	1.86	0.41
1:E:87:ILE:HB	1:E:225:GLU:OE1	2.19	0.41
2:F:39:ASP:HB3	2:F:41:ASN:HD21	1.85	0.41
2:F:8:THR:HB	1:G:4:THR:HB	2.02	0.41
1:G:123:THR:H	1:G:149:ASN:HD21	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:GLU:HG2	1:G:188:SER:OG	2.19	0.41
1:A:155:LYS:HB3	1:A:195:LEU:HD11	2.02	0.41
1:A:79:ILE:HB	1:A:226:THR:O	2.20	0.41
2:B:189:SER:O	2:B:190:LYS:HB2	2.21	0.41
2:D:21:LYS:HB2	2:D:21:LYS:HE2	1.78	0.41
1:E:22:GLN:NE2	1:E:51:ARG:HD3	2.35	0.41
1:C:252:PHE:HD1	1:C:253:LEU:HD22	1.86	0.41
1:E:92:ALA:O	1:E:213:PHE:HA	2.21	0.41
1:G:127:GLU:O	1:G:144:ILE:HA	2.21	0.41
2:H:95:LEU:HD13	2:H:124:VAL:CG2	2.49	0.41
1:A:155:LYS:HD3	1:A:195:LEU:CD1	2.51	0.41
2:D:105:GLY:O	2:D:108:PHE:CD2	2.70	0.41
2:D:67:VAL:HG11	2:D:240:PHE:O	2.21	0.41
1:G:184:LEU:O	1:G:192:SER:HA	2.21	0.41
1:C:117:PHE:HB2	1:C:150:SER:HB2	2.03	0.41
2:D:78:THR:OG1	2:D:230:PHE:HE1	2.04	0.41
1:G:13:LYS:O	1:G:14:PRO:C	2.58	0.41
1:G:8:THR:HG21	1:G:256:ASN:HA	2.02	0.41
2:H:97:PRO:HG3	2:H:122:GLN:HB2	2.03	0.41
1:A:194:ILE:HD13	2:B:192:SER:C	2.42	0.41
1:C:168:LYS:HG2	13:C:270:HOH:O	2.21	0.41
1:C:249:LEU:HD11	2:D:170:LEU:HD22	2.01	0.41
1:E:79:ILE:HD13	1:E:225:GLU:CG	2.51	0.41
1:E:48:SER:O	1:E:216:ALA:HA	2.21	0.41
1:E:49:LEU:HD11	1:E:103:LYS:O	2.20	0.41
2:H:213:PHE:CE2	2:H:232:TRP:CD2	3.09	0.41
2:B:39:ASP:HB2	2:B:40:LYS:CE	2.48	0.40
1:C:237:LYS:N	1:C:247:LEU:HD13	2.35	0.40
1:E:121:TYR:O	1:E:122:GLN:C	2.59	0.40
2:B:27:VAL:HA	2:B:32:THR:O	2.20	0.40
2:D:104:ALA:O	2:D:108:PHE:HB2	2.20	0.40
1:G:142:THR:CG2	13:G:259:HOH:O	2.67	0.40
1:A:49:LEU:CD1	1:A:105:GLY:HA3	2.51	0.40
1:C:252:PHE:CD1	1:C:253:LEU:N	2.89	0.40
2:D:173:TYR:CE2	2:D:201:LEU:HD22	2.56	0.40
1:E:91:LEU:HG	1:E:128:PHE:HB2	2.04	0.40
2:H:40:LYS:H	2:H:40:LYS:CE	2.34	0.40
2:H:88:ALA:HA	2:H:89:ASP:HA	1.90	0.40
1:A:167:ALA:HB2	1:A:186:TYR:CE1	2.56	0.40
2:D:79:ILE:HD12	2:D:226:THR:O	2.22	0.40
2:F:96:ALA:HB2	2:F:123:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:LEU:HD21	2:H:170:LEU:HD22	2.02	0.40
1:A:70:SER:OG	1:A:175:SER:HB2	2.22	0.40
2:B:201:LEU:HD12	2:B:201:LEU:HA	1.79	0.40
1:E:179:LEU:HD12	1:E:197:ASP:O	2.21	0.40
1:E:240:PHE:CZ	2:H:13:LYS:HE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/256 (96%)	229 (93%)	12 (5%)	5 (2%)	7	5
1	C	246/256 (96%)	230 (94%)	13 (5%)	3 (1%)	13	12
1	E	246/256 (96%)	228 (93%)	15 (6%)	3 (1%)	13	12
1	G	246/256 (96%)	231 (94%)	12 (5%)	3 (1%)	13	12
2	B	240/242 (99%)	227 (95%)	11 (5%)	2 (1%)	19	22
2	D	240/242 (99%)	224 (93%)	15 (6%)	1 (0%)	34	41
2	F	240/242 (99%)	230 (96%)	9 (4%)	1 (0%)	34	41
2	H	240/242 (99%)	226 (94%)	14 (6%)	0	100	100
All	All	1944/1992 (98%)	1825 (94%)	101 (5%)	18 (1%)	17	19

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	255	ALA
2	B	40	LYS
1	C	178	LYS
1	E	253	LEU

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Mol	Chain	Res	Type
1	E	255	ALA
2	D	189	SER
2	F	15	ASN
1	G	104	ALA
1	G	248	ASP
1	C	16	GLN
1	G	250	ALA
1	A	49	LEU
1	A	254	VAL
2	B	15	ASN
1	A	16	GLN
1	C	201	LEU
1	E	254	VAL

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	210/210 (100%)	175 (83%)	35 (17%)	2	1
1	C	210/210 (100%)	190 (90%)	20 (10%)	8	9
1	E	210/210 (100%)	173 (82%)	37 (18%)	2	1
1	G	210/210 (100%)	179 (85%)	31 (15%)	3	2
2	B	202/202 (100%)	177 (88%)	25 (12%)	4	4
2	D	202/202 (100%)	181 (90%)	21 (10%)	7	7
2	F	202/202 (100%)	178 (88%)	24 (12%)	5	4
2	H	202/202 (100%)	182 (90%)	20 (10%)	8	7
All	All	1648/1648 (100%)	1435 (87%)	213 (13%)	4	3

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	16	GLN

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Mol	Chain	Res	Type
1	A	19	LEU
1	A	20	LYS
1	A	21	LYS
1	A	33	LEU
1	A	35	LEU
1	A	36	THR
1	A	37	LYS
1	A	47	LYS
1	A	49	LEU
1	A	53	LEU
1	A	79	ILE
1	A	83	ASN
1	A	100	SER
1	A	119	SER
1	A	124	VAL
1	A	126	VAL
1	A	130	THR
1	A	172	THR
1	A	175	SER
1	A	179	LEU
1	A	190	LYS
1	A	194	ILE
1	A	198	VAL
1	A	199	VAL
1	A	201	LEU
1	A	209	VAL
1	A	220	SER
1	A	221	SER
1	A	224	ILE
1	A	247	LEU
1	A	253	LEU
1	A	254	VAL
1	A	256	ASN
2	B	2	THR
2	B	20	LYS
2	B	21	LYS
2	B	40	LYS
2	B	45	ASP
2	B	49	LEU
2	B	51	ARG
2	B	53	LEU
2	B	56	SER

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Mol	Chain	Res	Type
2	B	60	ILE
2	B	64	LYS
2	B	67	VAL
2	B	74	SER
2	B	79	ILE
2	B	84	ILE
2	B	86	THR
2	B	89	ASP
2	B	152	LYS
2	B	168	LYS
2	B	172	THR
2	B	180	LEU
2	B	190	LYS
2	B	192	SER
2	B	201	LEU
2	B	221	SER
1	C	1	THR
1	C	6	SER
1	C	21	LYS
1	C	40	LYS
1	C	49	LEU
1	C	53	LEU
1	C	59	ASN
1	C	60	ILE
1	C	64	LYS
1	C	95	LEU
1	C	98	VAL
1	C	99	SER
1	C	111	LEU
1	C	137	LEU
1	C	172	THR
1	C	199	VAL
1	C	202	LYS
1	C	238	LEU
1	C	249	LEU
1	C	256	ASN
2	D	2	THR
2	D	26	THR
2	D	27	VAL
2	D	36	THR
2	D	45	ASP
2	D	47	LYS

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Mol	Chain	Res	Type
2	D	53	LEU
2	D	56	SER
2	D	64	LYS
2	D	74	SER
2	D	76	ARG
2	D	89	ASP
2	D	134	THR
2	D	172	THR
2	D	189	SER
2	D	190	LYS
2	D	192	SER
2	D	201	LEU
2	D	205	LEU
2	D	221	SER
2	D	238	LEU
1	E	1	THR
1	E	6	SER
1	E	10	SER
1	E	18	ASN
1	E	20	LYS
1	E	21	LYS
1	E	22	GLN
1	E	27	VAL
1	E	29	SER
1	E	47	LYS
1	E	49	LEU
1	E	53	LEU
1	E	56	SER
1	E	64	LYS
1	E	79	ILE
1	E	89	ASP
1	E	91	LEU
1	E	116	VAL
1	E	117	PHE
1	E	119	SER
1	E	137	LEU
1	E	141	ASP
1	E	152	LYS
1	E	157	VAL
1	E	190	LYS
1	E	201	LEU
1	E	211	ILE

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Mol	Chain	Res	Type
1	E	220	SER
1	E	221	SER
1	E	224	ILE
1	E	226	THR
1	E	233	SER
1	E	237	LYS
1	E	247	LEU
1	E	248	ASP
1	E	254	VAL
1	E	256	ASN
2	F	2	THR
2	F	19	LEU
2	F	21	LYS
2	F	30	SER
2	F	35	LEU
2	F	40	LYS
2	F	41	ASN
2	F	43	VAL
2	F	47	LYS
2	F	49	LEU
2	F	51	ARG
2	F	68	VAL
2	F	89	ASP
2	F	91	LEU
2	F	98	VAL
2	F	99	SER
2	F	103	LYS
2	F	123	THR
2	F	137	LEU
2	F	168	LYS
2	F	201	LEU
2	F	211	ILE
2	F	221	SER
2	F	237	LYS
1	G	2	THR
1	G	4	THR
1	G	6	SER
1	G	8	THR
1	G	11	LYS
1	G	21	LYS
1	G	26	THR
1	G	30	SER

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Mol	Chain	Res	Type
1	G	33	LEU
1	G	35	LEU
1	G	36	THR
1	G	47	LYS
1	G	49	LEU
1	G	64	LYS
1	G	68	VAL
1	G	79	ILE
1	G	89	ASP
1	G	98	VAL
1	G	99	SER
1	G	108	PHE
1	G	111	LEU
1	G	141	ASP
1	G	148	VAL
1	G	165	GLU
1	G	176	SER
1	G	190	LYS
1	G	201	LEU
1	G	202	LYS
1	G	205	LEU
1	G	251	SER
1	G	252	PHE
2	H	6	SER
2	H	21	LYS
2	H	26	THR
2	H	37	LYS
2	H	40	LYS
2	H	43	VAL
2	H	49	LEU
2	H	64	LYS
2	H	79	ILE
2	H	84	ILE
2	H	103	LYS
2	H	111	LEU
2	H	124	VAL
2	H	132	GLU
2	H	191	THR
2	H	205	LEU
2	H	207	GLU
2	H	221	SER
2	H	237	LYS

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Mol	Chain	Res	Type
2	H	238	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	15	ASN
1	A	59	ASN
1	A	83	ASN
1	A	149	ASN
1	A	227	HIS
2	B	3	ASN
2	B	59	ASN
2	B	149	ASN
2	B	227	HIS
1	C	16	GLN
1	C	149	ASN
1	C	227	HIS
2	D	59	ASN
2	D	227	HIS
1	E	18	ASN
1	E	22	GLN
1	E	59	ASN
1	E	227	HIS
1	E	256	ASN
2	F	18	ASN
2	F	22	GLN
2	F	41	ASN
2	F	59	ASN
2	F	149	ASN
2	F	227	HIS
1	G	3	ASN
1	G	59	ASN
1	G	149	ASN
2	H	16	GLN
2	H	59	ASN
2	H	149	ASN
2	H	227	HIS

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 ⓘ

21 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	I	1	1,3	14,14,15	0.71	1 (7%)	17,19,21	1.51	3 (17%)
3	NAG	I	2	3	14,14,15	0.59	0	17,19,21	2.18	4 (23%)
3	BMA	I	3	3	11,11,12	1.30	3 (27%)	15,15,17	2.36	5 (33%)
3	FUC	I	4	3	10,10,11	0.73	0	14,14,16	1.52	3 (21%)
4	NAG	J	1	2,4	14,14,15	0.89	1 (7%)	17,19,21	2.35	3 (17%)
4	NAG	J	2	4	14,14,15	1.05	1 (7%)	17,19,21	1.98	4 (23%)
4	BMA	J	3	4	11,11,12	2.32	3 (27%)	15,15,17	4.21	6 (40%)
4	MAN	J	4	4	11,11,12	6.34	8 (72%)	15,15,17	3.98	8 (53%)
4	FUC	J	5	4	10,10,11	0.75	0	14,14,16	1.27	3 (21%)
3	NAG	K	1	1,3	14,14,15	0.58	0	17,19,21	1.35	2 (11%)
3	NAG	K	2	3	14,14,15	0.59	0	17,19,21	1.60	5 (29%)
3	BMA	K	3	3	11,11,12	0.81	0	15,15,17	1.14	1 (6%)
3	FUC	K	4	3	10,10,11	4.32	4 (40%)	14,14,16	4.37	5 (35%)
3	NAG	L	1	1,3	14,14,15	1.18	2 (14%)	17,19,21	1.62	4 (23%)
3	NAG	L	2	3	14,14,15	0.71	0	17,19,21	2.31	7 (41%)
3	BMA	L	3	3	11,11,12	0.81	0	15,15,17	1.45	3 (20%)
3	FUC	L	4	3	10,10,11	0.80	0	14,14,16	1.00	1 (7%)
5	NAG	M	1	1,5	14,14,15	0.71	0	17,19,21	1.49	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	M	2	5	14,14,15	0.87	1 (7%)	17,19,21	1.93	4 (23%)
6	NAG	N	1	2,6	14,14,15	1.41	3 (21%)	17,19,21	2.69	6 (35%)
6	FUC	N	2	6	10,10,11	3.78	4 (40%)	14,14,16	4.08	8 (57%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	FUC	I	4	3	-	-	0/1/1/1
4	NAG	J	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	1/2/19/22	0/1/1/1
4	MAN	J	4	4	-	2/2/19/22	0/1/1/1
4	FUC	J	5	4	-	-	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	1/2/19/22	0/1/1/1
3	FUC	K	4	3	-	-	0/1/1/1
3	NAG	L	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	2/2/19/22	0/1/1/1
3	FUC	L	4	3	-	-	0/1/1/1
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
6	NAG	N	1	2,6	-	1/6/23/26	0/1/1/1
6	FUC	N	2	6	-	-	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	4	FUC	C2-C3	-12.58	1.34	1.52
4	J	4	MAN	O5-C5	-12.03	1.19	1.43
4	J	4	MAN	C2-C3	-9.27	1.38	1.52
4	J	4	MAN	O2-C2	8.96	1.62	1.43
6	N	2	FUC	C4-C5	-7.19	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	4	MAN	C1-C2	-6.95	1.36	1.52
6	N	2	FUC	C2-C3	6.67	1.62	1.52
4	J	4	MAN	C4-C5	-6.16	1.40	1.53
6	N	2	FUC	O3-C3	5.66	1.56	1.43
4	J	4	MAN	O3-C3	-4.79	1.31	1.43
4	J	3	BMA	O3-C3	-4.70	1.31	1.43
4	J	3	BMA	O4-C4	-3.87	1.33	1.43
4	J	3	BMA	C2-C3	3.58	1.57	1.52
4	J	4	MAN	C4-C3	3.53	1.61	1.52
3	K	4	FUC	C6-C5	3.32	1.59	1.51
4	J	1	NAG	O5-C1	-3.10	1.38	1.43
6	N	1	NAG	C4-C3	-3.05	1.44	1.52
6	N	1	NAG	O5-C1	2.98	1.48	1.43
4	J	4	MAN	O5-C1	-2.81	1.39	1.43
3	L	1	NAG	O5-C1	-2.74	1.39	1.43
6	N	2	FUC	O5-C5	2.70	1.49	1.43
3	L	1	NAG	C4-C5	2.60	1.58	1.53
3	I	3	BMA	O5-C1	2.26	1.47	1.43
6	N	1	NAG	C3-C2	-2.26	1.47	1.52
4	J	2	NAG	C2-N2	-2.20	1.42	1.46
3	K	4	FUC	O3-C3	-2.16	1.37	1.43
3	K	4	FUC	O4-C4	2.15	1.48	1.43
3	I	3	BMA	C2-C3	2.13	1.55	1.52
5	M	2	NAG	C4-C5	-2.09	1.48	1.53
3	I	3	BMA	O5-C5	2.04	1.47	1.43
3	I	1	NAG	O5-C1	-2.03	1.40	1.43

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	4	FUC	C1-C2-C3	12.71	125.29	109.67
4	J	3	BMA	O4-C4-C5	11.56	138.01	109.30
6	N	2	FUC	C6-C5-C4	10.45	132.39	113.07
4	J	3	BMA	O3-C3-C2	9.83	128.82	109.99
4	J	4	MAN	C1-C2-C3	8.28	119.84	109.67
4	J	1	NAG	C1-O5-C5	7.57	122.45	112.19
6	N	1	NAG	C1-O5-C5	7.04	121.73	112.19
3	K	4	FUC	O5-C5-C4	6.83	121.78	109.52
3	I	3	BMA	O5-C5-C6	6.60	117.56	107.20
4	J	4	MAN	O5-C5-C4	6.23	125.99	110.83
4	J	4	MAN	O3-C3-C4	-6.22	95.97	110.35
3	I	2	NAG	C1-O5-C5	6.14	120.51	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	2	NAG	C1-C2-N2	-6.10	100.07	110.49
6	N	2	FUC	O3-C3-C2	-5.97	98.57	109.99
6	N	2	FUC	O4-C4-C5	-5.08	98.41	109.67
6	N	2	FUC	C3-C4-C5	4.92	117.43	109.77
4	J	2	NAG	O4-C4-C3	-4.87	99.08	110.35
4	J	4	MAN	O4-C4-C5	4.85	121.34	109.30
4	J	4	MAN	C3-C4-C5	-4.80	101.67	110.24
3	K	4	FUC	O2-C2-C3	4.58	119.31	110.14
5	M	2	NAG	C1-O5-C5	4.50	118.29	112.19
3	L	1	NAG	O5-C5-C6	-4.20	100.62	107.20
6	N	1	NAG	O5-C5-C6	-3.97	100.98	107.20
5	M	2	NAG	O4-C4-C5	3.97	119.15	109.30
3	K	4	FUC	C6-C5-C4	-3.90	105.87	113.07
5	M	1	NAG	C2-N2-C7	3.73	128.22	122.90
6	N	1	NAG	C2-N2-C7	3.72	128.20	122.90
4	J	4	MAN	O2-C2-C3	-3.62	102.89	110.14
6	N	1	NAG	C4-C3-C2	3.60	116.29	111.02
3	L	2	NAG	C1-O5-C5	-3.53	107.41	112.19
4	J	2	NAG	C1-C2-N2	-3.48	104.55	110.49
3	I	1	NAG	C3-C4-C5	-3.45	104.08	110.24
3	I	2	NAG	O5-C5-C6	-3.41	101.86	107.20
3	L	2	NAG	C2-N2-C7	3.30	127.60	122.90
4	J	4	MAN	C1-O5-C5	3.29	116.64	112.19
3	K	2	NAG	O4-C4-C3	-3.18	102.99	110.35
4	J	3	BMA	O3-C3-C4	-3.08	103.24	110.35
3	L	3	BMA	C1-O5-C5	3.07	116.35	112.19
3	I	2	NAG	C6-C5-C4	-3.06	105.84	113.00
4	J	3	BMA	C3-C4-C5	-3.00	104.88	110.24
3	I	4	FUC	O5-C5-C6	2.98	113.74	107.33
4	J	2	NAG	C8-C7-N2	-2.86	111.25	116.10
3	L	1	NAG	C1-O5-C5	2.83	116.03	112.19
3	I	3	BMA	C6-C5-C4	-2.81	106.41	113.00
3	I	4	FUC	O5-C1-C2	-2.81	106.43	110.77
4	J	4	MAN	O6-C6-C5	-2.79	101.71	111.29
3	K	1	NAG	O5-C1-C2	2.79	115.69	111.29
5	M	1	NAG	C1-C2-N2	-2.79	105.73	110.49
3	K	4	FUC	O4-C4-C3	-2.76	103.96	110.35
6	N	2	FUC	O4-C4-C3	2.73	116.65	110.35
5	M	2	NAG	C3-C4-C5	2.71	115.08	110.24
6	N	2	FUC	C1-C2-C3	-2.69	106.36	109.67
6	N	1	NAG	O3-C3-C4	2.68	116.55	110.35
3	I	3	BMA	C2-C3-C4	2.67	115.52	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	NAG	O6-C6-C5	-2.61	102.33	111.29
6	N	2	FUC	C1-O5-C5	2.58	118.62	112.78
3	K	2	NAG	C2-N2-C7	2.51	126.47	122.90
3	K	1	NAG	C2-N2-C7	2.44	126.38	122.90
3	L	2	NAG	O5-C1-C2	-2.44	107.44	111.29
3	L	3	BMA	O5-C5-C6	2.41	110.98	107.20
5	M	1	NAG	O3-C3-C2	2.38	114.39	109.47
3	I	1	NAG	C1-C2-N2	2.38	114.55	110.49
4	J	1	NAG	O5-C1-C2	2.37	115.03	111.29
6	N	1	NAG	O7-C7-N2	2.36	126.28	121.95
4	J	2	NAG	C4-C3-C2	-2.35	107.57	111.02
3	I	4	FUC	O2-C2-C1	2.33	113.92	109.15
3	I	3	BMA	O5-C1-C2	2.32	114.35	110.77
3	I	2	NAG	C3-C4-C5	2.31	114.36	110.24
3	L	2	NAG	C4-C3-C2	-2.25	107.71	111.02
3	L	4	FUC	C1-O5-C5	2.22	117.80	112.78
4	J	5	FUC	C2-C3-C4	2.21	114.71	110.89
3	K	2	NAG	O5-C1-C2	2.17	114.72	111.29
4	J	3	BMA	O4-C4-C3	-2.16	105.36	110.35
4	J	3	BMA	C1-O5-C5	2.14	115.09	112.19
4	J	5	FUC	C1-O5-C5	2.13	117.61	112.78
3	I	3	BMA	C3-C4-C5	2.13	114.04	110.24
3	L	1	NAG	O4-C4-C3	-2.13	105.43	110.35
3	L	2	NAG	C8-C7-N2	2.11	119.68	116.10
3	L	1	NAG	O6-C6-C5	-2.10	104.09	111.29
4	J	5	FUC	C3-C4-C5	2.09	113.03	109.77
3	L	3	BMA	C1-C2-C3	-2.09	107.10	109.67
4	J	1	NAG	C6-C5-C4	-2.09	108.12	113.00
3	L	2	NAG	O3-C3-C4	-2.05	105.62	110.35
3	K	3	BMA	O5-C5-C6	2.04	110.41	107.20
6	N	2	FUC	C2-C3-C4	2.04	114.42	110.89
3	K	2	NAG	C1-C2-N2	-2.02	107.03	110.49
3	K	2	NAG	C1-O5-C5	2.00	114.90	112.19
5	M	2	NAG	C2-N2-C7	2.00	125.75	122.90

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	L	3	BMA	C4-C5-C6-O6

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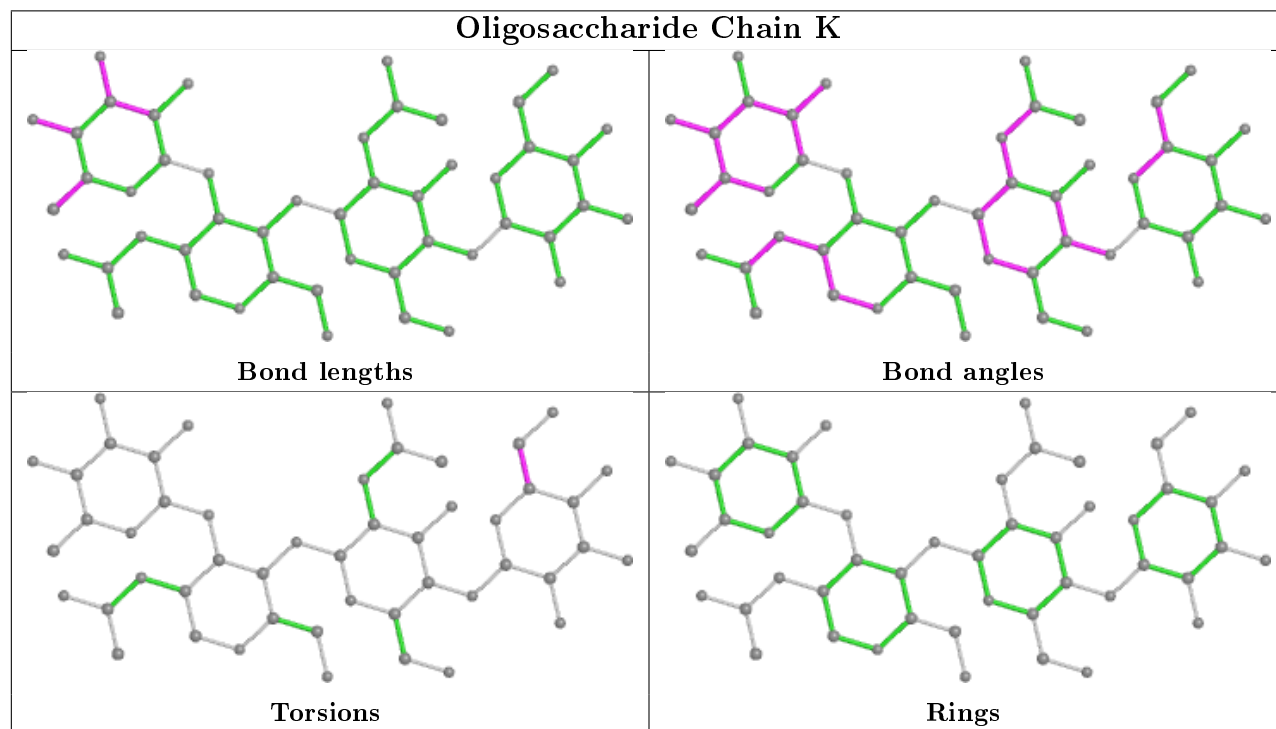
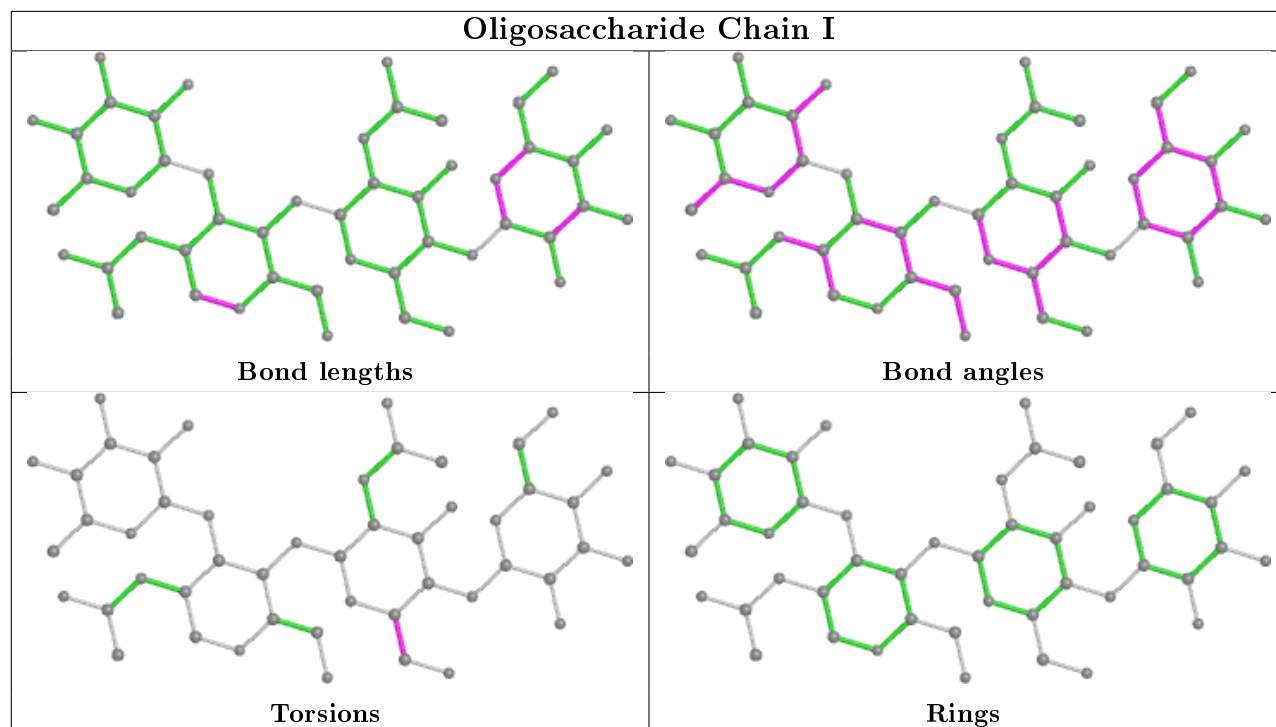
Mol	Chain	Res	Type	Atoms
4	J	1	NAG	C4-C5-C6-O6
4	J	4	MAN	C4-C5-C6-O6
3	L	2	NAG	C8-C7-N2-C2
3	L	2	NAG	O7-C7-N2-C2
4	J	1	NAG	O5-C5-C6-O6
4	J	4	MAN	O5-C5-C6-O6
3	L	3	BMA	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6

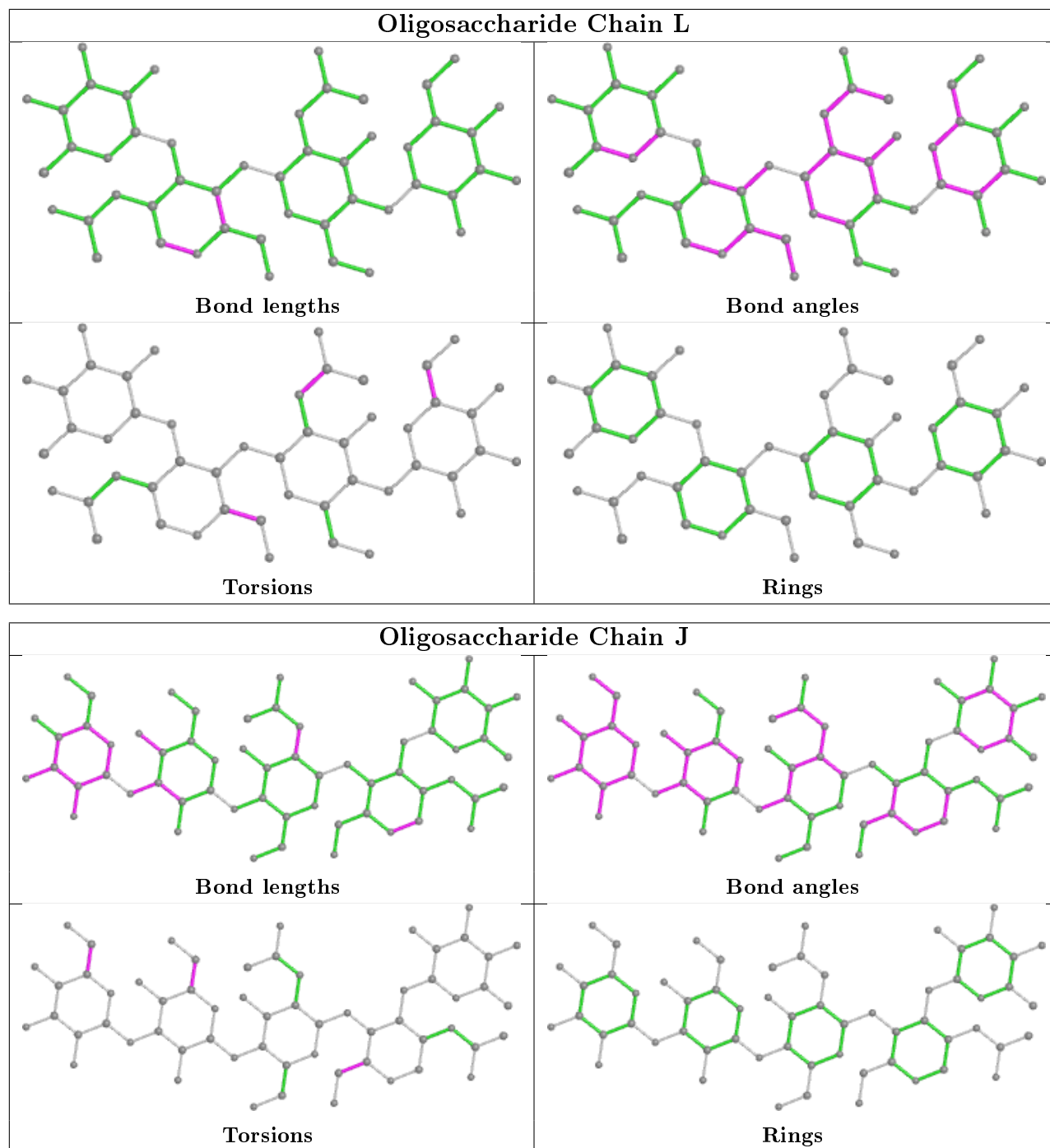
There are no ring outliers.

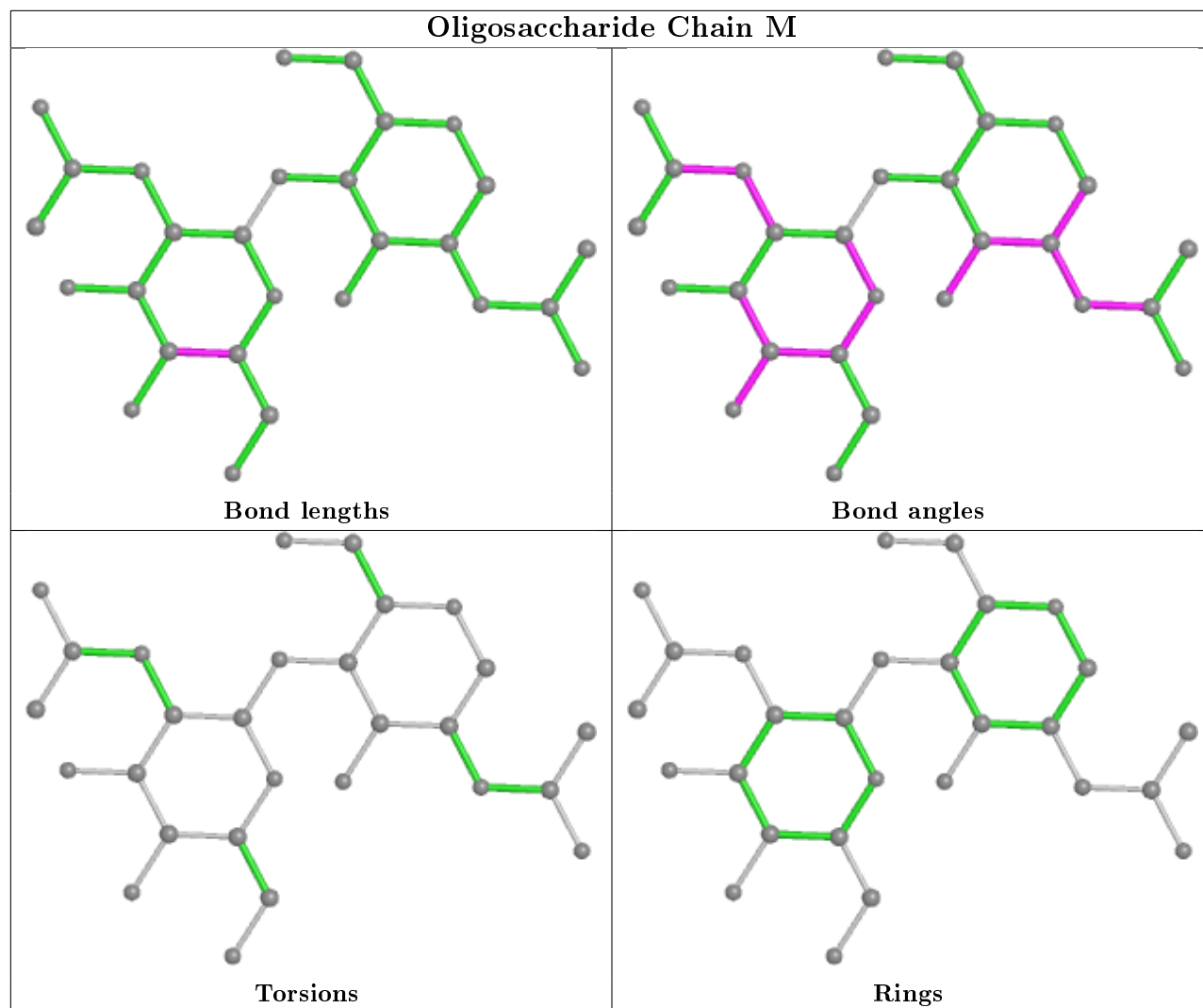
9 monomers are involved in 14 short contacts:

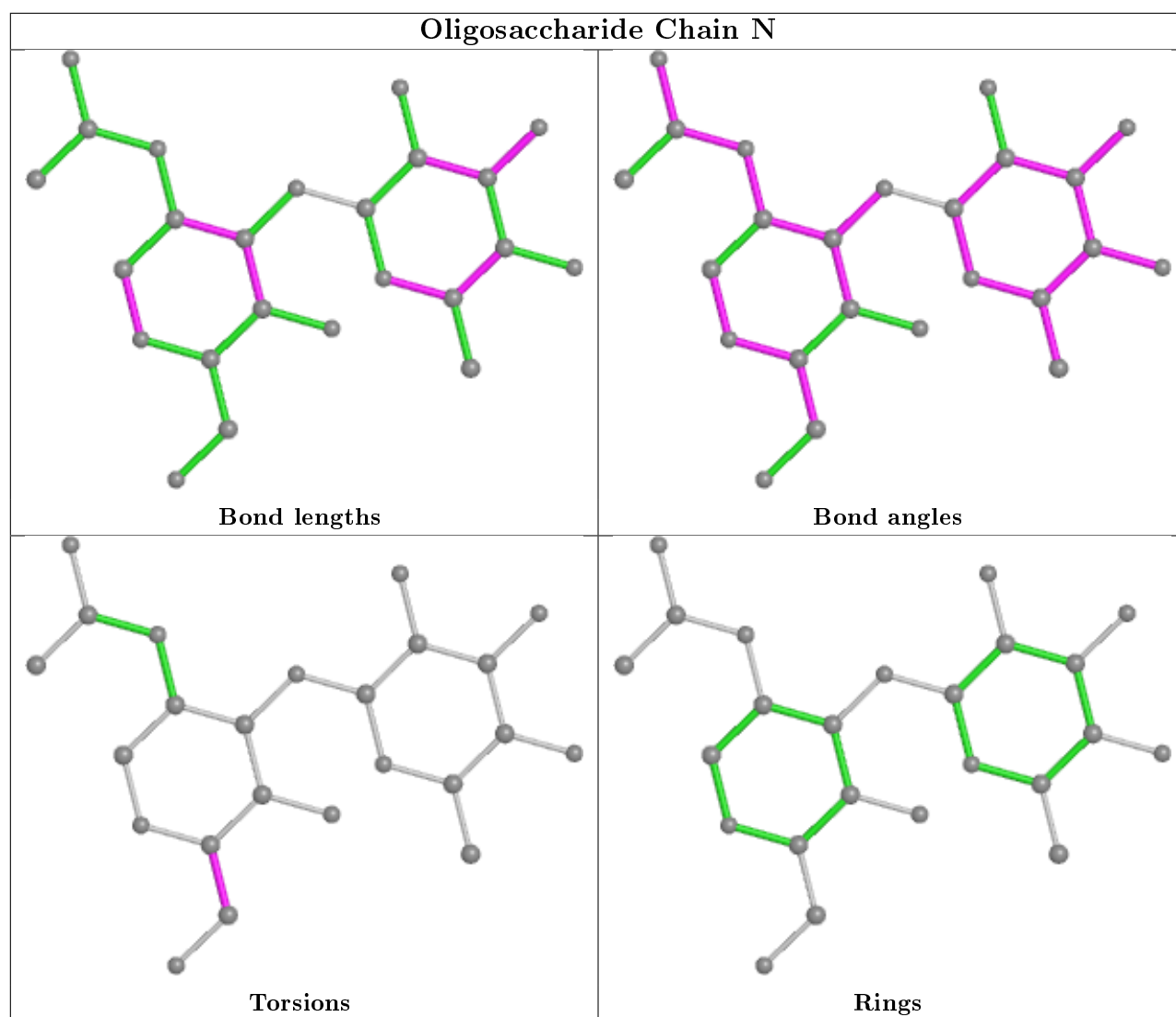
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	4	FUC	1	0
4	J	1	NAG	1	0
3	I	1	NAG	2	0
4	J	3	BMA	8	0
3	I	2	NAG	2	0
3	I	3	BMA	1	0
3	I	4	FUC	1	0
4	J	4	MAN	2	0
3	L	2	NAG	1	0

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](#)

Of 34 ligands modelled in this entry, 16 are monoatomic - leaving 18 for Mogul analysis.

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	$\# Z > 2$
9	ABU	G	286	-	3,6,6	0.35	0	2,6,6	0.36	0
10	GOL	B	281	-	5,5,5	0.29	0	5,5,5	0.92	0
9	ABU	D	278	-	3,6,6	0.22	0	2,6,6	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GOL	C	283	-	5,5,5	0.35	0	5,5,5	0.70	0
9	ABU	A	280	-	3,6,6	0.29	0	2,6,6	0.56	0
10	GOL	G	287	-	5,5,5	0.31	0	5,5,5	0.32	0
10	GOL	E	279	-	5,5,5	0.27	0	5,5,5	1.14	1 (20%)
9	ABU	B	276	-	3,6,6	0.39	0	2,6,6	0.13	0
10	GOL	E	291	-	5,5,5	0.42	0	5,5,5	0.64	0
9	ABU	E	284	-	3,6,6	0.59	0	2,6,6	0.53	0
9	ABU	F	290	-	3,6,6	0.39	0	2,6,6	1.72	1 (50%)
10	GOL	A	277	-	5,5,5	0.28	0	5,5,5	0.60	0
10	GOL	D	285	-	5,5,5	0.32	0	5,5,5	0.65	0
11	XYP	B	306	-	9,9,10	2.45	3 (33%)	10,12,14	6.50	5 (50%)
9	ABU	E	288	-	3,6,6	0.14	0	2,6,6	0.58	0
10	GOL	H	289	-	5,5,5	0.31	0	5,5,5	0.43	0
9	ABU	C	282	-	3,6,6	0.25	0	2,6,6	0.08	0
12	NAG	D	301	2	14,14,15	1.81	3 (21%)	17,19,21	1.64	4 (23%)

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
9	ABU	G	286	-	-	2/2/4/4	-
10	GOL	B	281	-	-	0/4/4/4	-
9	ABU	D	278	-	-	2/2/4/4	-
10	GOL	C	283	-	-	0/4/4/4	-
9	ABU	A	280	-	-	1/2/4/4	-
10	GOL	G	287	-	-	2/4/4/4	-
10	GOL	E	279	-	-	2/4/4/4	-
9	ABU	B	276	-	-	1/2/4/4	-
10	GOL	E	291	-	-	4/4/4/4	-
9	ABU	E	284	-	-	0/2/4/4	-
9	ABU	F	290	-	-	1/2/4/4	-
10	GOL	A	277	-	-	2/4/4/4	-
10	GOL	D	285	-	-	4/4/4/4	-
11	XYP	B	306	-	-	-	0/1/1/1
9	ABU	E	288	-	-	1/2/4/4	-
10	GOL	H	289	-	-	2/4/4/4	-
9	ABU	C	282	-	-	1/2/4/4	-
12	NAG	D	301	2	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	306	XYP	O5-C1	5.75	1.54	1.42
12	D	301	NAG	C1-C2	-4.27	1.46	1.52
12	D	301	NAG	C3-C2	-4.03	1.43	1.52
11	B	306	XYP	C5-C4	2.91	1.58	1.52
11	B	306	XYP	C4-C3	2.80	1.56	1.52
12	D	301	NAG	C2-N2	2.76	1.51	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	306	XYP	C1-C2-C3	16.27	129.67	109.67
11	B	306	XYP	C5-O5-C1	9.43	126.02	111.52
11	B	306	XYP	O4-C4-C3	-6.03	98.05	110.14
11	B	306	XYP	O4-C4-C5	-4.76	99.42	109.15
12	D	301	NAG	C1-O5-C5	4.14	117.80	112.19
12	D	301	NAG	O3-C3-C2	3.08	115.84	109.47
12	D	301	NAG	C2-N2-C7	-2.45	119.41	122.90
11	B	306	XYP	O3-C3-C2	-2.44	105.32	109.99
9	F	290	ABU	CA-CB-CG	-2.27	106.11	112.84
10	E	279	GOL	O3-C3-C2	-2.20	99.64	110.20
12	D	301	NAG	C1-C2-N2	2.13	114.12	110.49

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	H	289	GOL	O1-C1-C2-C3
10	A	277	GOL	C1-C2-C3-O3
9	E	288	ABU	CA-CB-CG-CD
10	G	287	GOL	O1-C1-C2-C3
10	D	285	GOL	O1-C1-C2-C3
10	D	285	GOL	C1-C2-C3-O3
10	E	291	GOL	O1-C1-C2-C3
10	E	279	GOL	O1-C1-C2-C3
12	D	301	NAG	O5-C5-C6-O6
12	D	301	NAG	C4-C5-C6-O6
10	E	279	GOL	O1-C1-C2-O2
10	E	291	GOL	C1-C2-C3-O3
10	H	289	GOL	O1-C1-C2-O2
10	D	285	GOL	O2-C2-C3-O3
10	E	291	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
9	G	286	ABU	CA-CB-CG-CD
10	A	277	GOL	O2-C2-C3-O3
10	G	287	GOL	O1-C1-C2-O2
9	D	278	ABU	N-CA-CB-CG
10	D	285	GOL	O1-C1-C2-O2
9	C	282	ABU	CA-CB-CG-CD
9	D	278	ABU	CA-CB-CG-CD
9	G	286	ABU	N-CA-CB-CG
10	E	291	GOL	O2-C2-C3-O3
9	A	280	ABU	N-CA-CB-CG
9	F	290	ABU	N-CA-CB-CG
9	B	276	ABU	N-CA-CB-CG

There are no ring outliers.

13 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	G	286	ABU	1	0
9	D	278	ABU	1	0
10	C	283	GOL	1	0
9	A	280	ABU	5	0
10	E	279	GOL	2	0
9	B	276	ABU	6	0
9	E	284	ABU	3	0
9	F	290	ABU	7	0
10	A	277	GOL	2	0
11	B	306	XYP	6	0
9	E	288	ABU	8	0
10	H	289	GOL	3	0
9	C	282	ABU	6	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	250/256 (97%)	-0.02	1 (0%) 92 93	12, 20, 30, 48	1 (0%)
1	C	250/256 (97%)	-0.03	4 (1%) 72 69	12, 21, 39, 63	0
1	E	250/256 (97%)	0.22	8 (3%) 47 44	14, 24, 40, 59	0
1	G	250/256 (97%)	-0.05	2 (0%) 86 86	14, 22, 35, 52	0
2	B	242/242 (100%)	-0.05	1 (0%) 92 93	11, 18, 26, 35	2 (0%)
2	D	242/242 (100%)	0.11	5 (2%) 63 60	15, 26, 41, 58	0
2	F	242/242 (100%)	-0.15	3 (1%) 79 77	14, 19, 28, 50	1 (0%)
2	H	242/242 (100%)	0.03	5 (2%) 63 60	17, 26, 39, 55	0
All	All	1968/1992 (98%)	0.01	29 (1%) 73 71	11, 22, 38, 63	4 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	255	ALA	5.8
2	H	241	ALA	4.6
1	E	247	LEU	4.3
2	F	241	ALA	4.1
1	E	255	ALA	3.9
2	F	242	ALA	3.6
2	D	242	ALA	3.4
1	E	43	VAL	3.4
2	D	101	PRO	3.1
1	E	40	LYS	2.9
2	D	241	ALA	2.9
1	C	251	SER	2.8
2	D	100	SER	2.8
2	H	101	PRO	2.7
2	D	116	VAL	2.7
1	E	38	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	80	TYR	2.5
2	H	242	ALA	2.4
1	C	176	SER	2.3
1	C	100	SER	2.2
1	E	15	ASN	2.2
1	E	41	ASN	2.2
2	H	40	LYS	2.1
1	C	15	ASN	2.1
1	G	247	LEU	2.1
1	A	100	SER	2.1
2	F	15	ASN	2.0
2	B	1	THR	2.0
2	H	67	VAL	2.0

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.

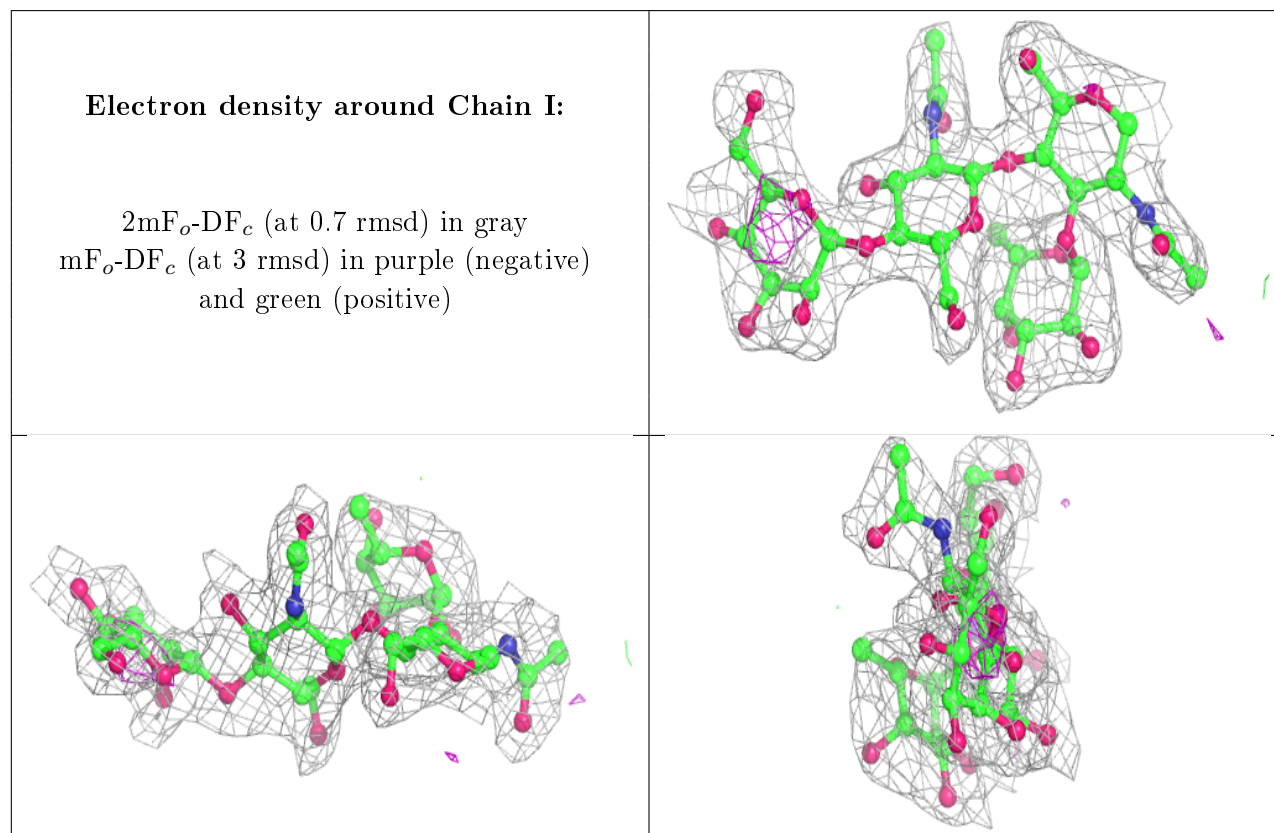
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	I	3	11/12	0.58	0.26	39,42,44,46	0
5	NAG	M	2	14/15	0.69	0.33	60,70,79,81	0
3	BMA	L	3	11/12	0.72	0.19	42,46,48,49	0
6	FUC	N	2	10/11	0.76	0.27	60,63,68,70	0
3	BMA	K	3	11/12	0.79	0.15	42,46,48,48	0
4	BMA	J	3	11/12	0.81	0.17	34,38,39,42	0
4	MAN	J	4	11/12	0.83	0.23	39,41,44,45	0
5	NAG	M	1	14/15	0.89	0.21	44,52,59,60	0
6	NAG	N	1	14/15	0.89	0.14	40,46,48,55	0
3	NAG	K	2	14/15	0.90	0.17	36,39,42,42	0
3	NAG	K	1	14/15	0.90	0.14	28,32,33,35	0
4	NAG	J	1	14/15	0.93	0.13	20,22,25,25	0
3	NAG	L	1	14/15	0.93	0.15	24,26,28,30	0
3	FUC	L	4	10/11	0.94	0.13	28,30,32,32	0
4	FUC	J	5	10/11	0.94	0.15	25,27,29,30	0

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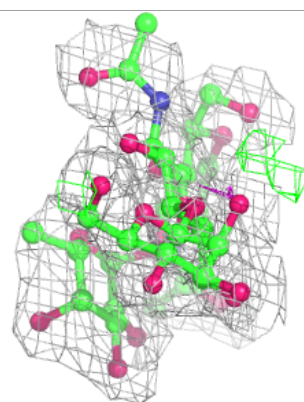
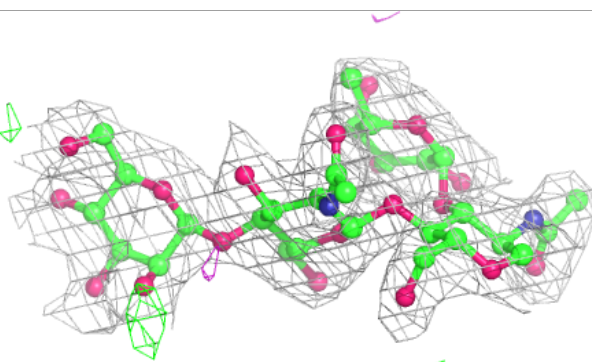
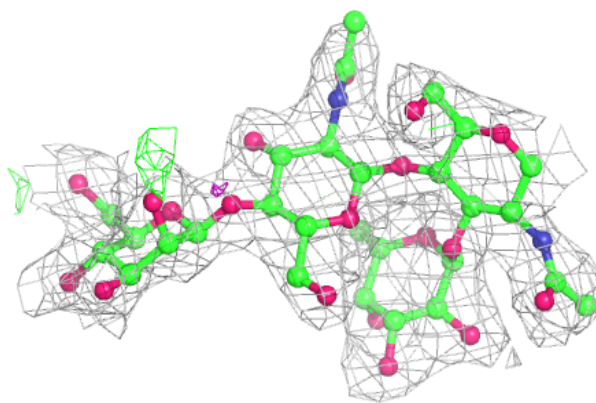
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	I	2	14/15	0.94	0.12	32,33,36,37	0
3	NAG	L	2	14/15	0.94	0.10	32,34,38,40	0
3	FUC	I	4	10/11	0.95	0.18	33,35,37,37	0
3	NAG	I	1	14/15	0.95	0.14	26,29,31,32	0
3	FUC	K	4	10/11	0.95	0.09	32,34,35,36	0
4	NAG	J	2	14/15	0.97	0.13	26,28,31,32	0

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.

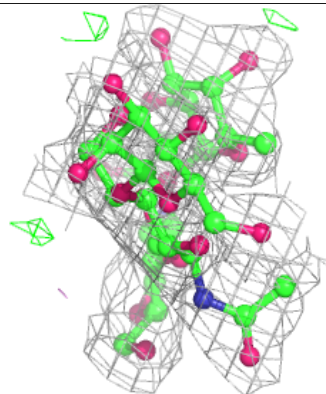
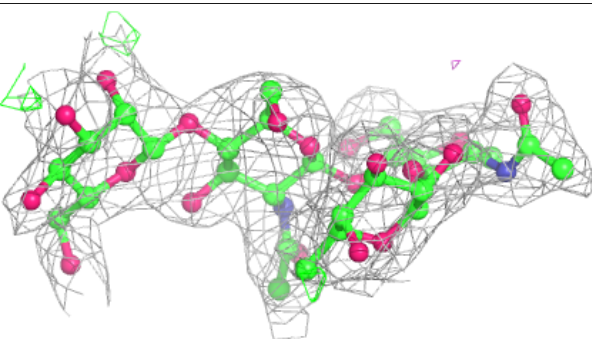
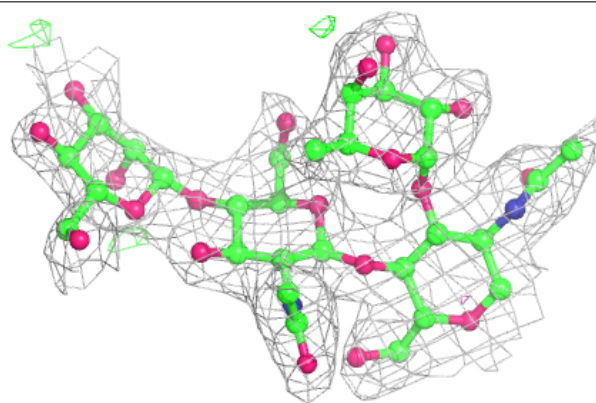


Electron density around Chain K:

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

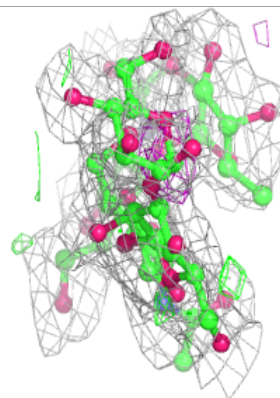
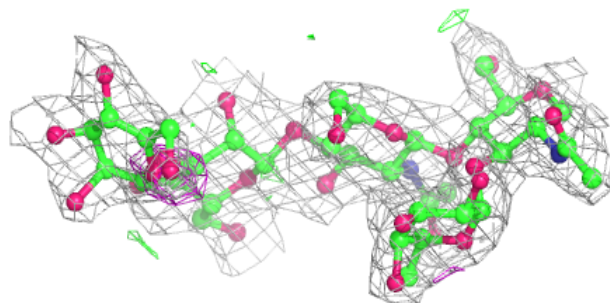
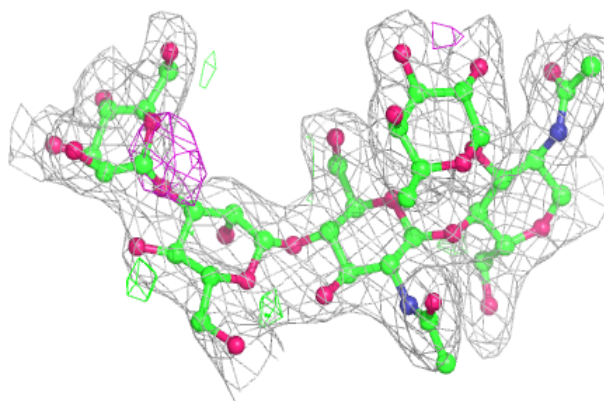
**Electron density around Chain L:**

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



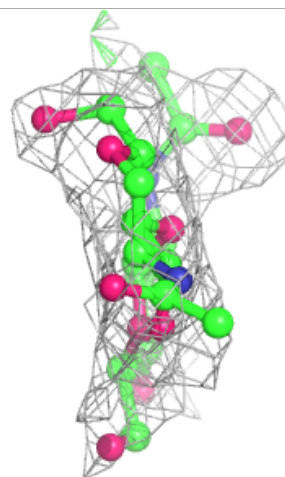
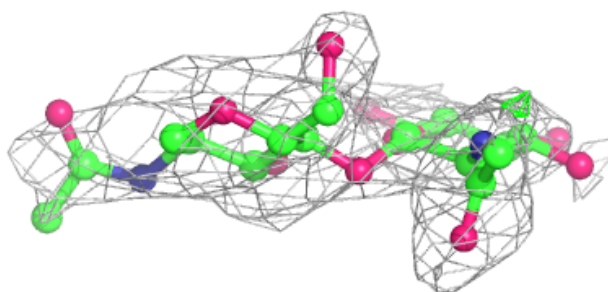
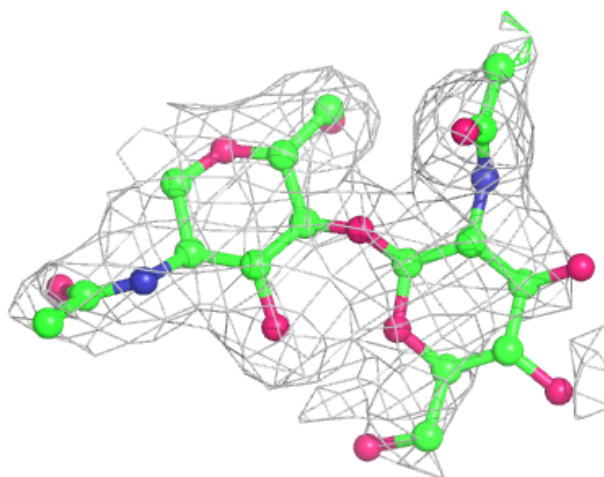
Electron density around Chain J:

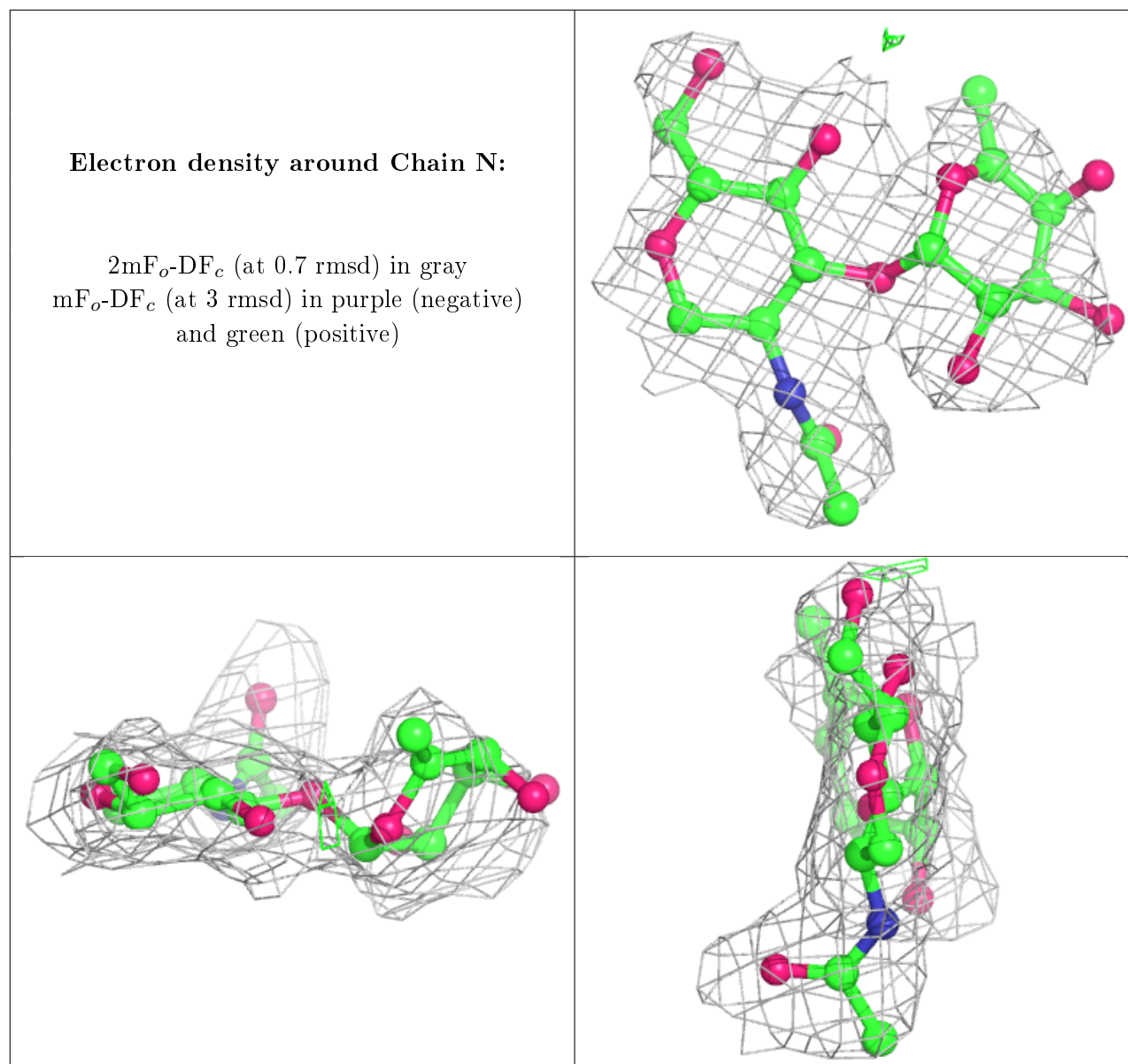
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain M:

$2mF_o-DF_c$ (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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	NAG	D	301	14/15	0.77	0.23	50,56,59,60	0
11	XYP	B	306	9/10	0.85	0.17	41,41,43,43	0
9	ABU	E	284	7/7	0.88	0.26	25,28,33,33	0
10	GOL	D	285	6/6	0.89	0.20	32,33,33,34	0
10	GOL	A	277	6/6	0.90	0.18	30,33,34,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	GOL	H	289	6/6	0.90	0.15	29,31,31,34	0
9	ABU	D	278	7/7	0.91	0.29	29,30,33,35	0
9	ABU	B	276	7/7	0.92	0.31	27,30,34,35	0
9	ABU	E	288	7/7	0.92	0.38	32,36,38,38	0
10	GOL	E	291	6/6	0.93	0.13	29,29,31,33	0
10	GOL	E	279	6/6	0.93	0.19	31,32,33,35	0
9	ABU	F	290	7/7	0.93	0.28	14,16,20,22	0
10	GOL	C	283	6/6	0.93	0.17	25,25,26,26	0
9	ABU	C	282	7/7	0.94	0.29	29,30,33,34	0
9	ABU	A	280	7/7	0.94	0.20	22,24,27,28	0
10	GOL	G	287	6/6	0.95	0.14	29,29,30,31	0
9	ABU	G	286	7/7	0.95	0.27	31,33,35,37	0
10	GOL	B	281	6/6	0.95	0.13	20,21,22,23	0
7	CA	F	274	1/1	0.96	0.07	23,23,23,23	0
7	CA	H	272	1/1	0.97	0.11	30,30,30,30	0
7	CA	D	268	1/1	0.97	0.08	31,31,31,31	0
8	MN	C	267	1/1	0.98	0.09	20,20,20,20	0
8	MN	E	263	1/1	0.98	0.06	25,25,25,25	0
8	MN	H	273	1/1	0.98	0.09	23,23,23,23	0
7	CA	G	270	1/1	0.99	0.05	17,17,17,17	0
8	MN	B	261	1/1	0.99	0.07	13,13,13,13	0
7	CA	C	266	1/1	0.99	0.10	19,19,19,19	0
7	CA	E	262	1/1	0.99	0.06	20,20,20,20	0
8	MN	F	275	1/1	0.99	0.07	21,21,21,21	0
7	CA	A	264	1/1	0.99	0.09	19,19,19,19	0
8	MN	D	269	1/1	0.99	0.04	38,38,38,38	0
8	MN	A	265	1/1	1.00	0.10	13,13,13,13	0
7	CA	B	260	1/1	1.00	0.10	15,15,15,15	0
8	MN	G	271	1/1	1.00	0.06	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.