Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:58 AM BST

PDB ID	:	3SAJ
Title	:	Crystal Structure of glutamate receptor GluA1 Amino Terminal Domain
Authors	:	Jin, R.; Zong, Y.; Yao, G.; Gu, S.
Deposited on	:	2011-06-02
Resolution	:	2.50 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:

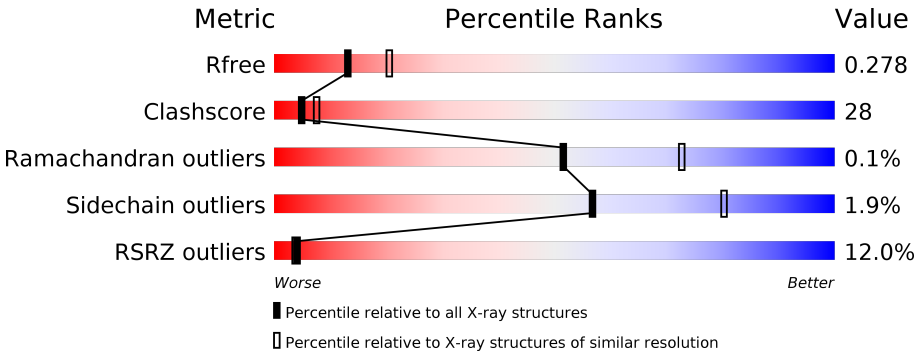
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	384	9% 65% 30%
1	B	384	12% 61% 33% 5%
1	C	384	15% 58% 37%
1	D	384	10% 61% 32%
2	E	3	67% 33%
2	H	3	67% 33%

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Mol	Chain	Length	Quality of chain
2	N	3	67% 33%
3	F	2	50% 50%
3	G	2	50% 50%
3	I	2	50% 50%
3	J	2	100%
3	K	2	100%
3	L	2	100%
3	O	2	100%
3	P	2	100%
4	M	7	14% 57% 29%

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
3	NAG	I	2	-	-	-	X
3	NAG	O	2	-	-	-	X
4	MAN	M	5	-	-	-	X
4	MAN	M	6	-	-	-	X
5	NAG	D	900	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12534 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 Glutamate receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	1	0
			2987	1899	525	550	13			
1	B	366	Total	C	N	O	S	0	0	0
			2959	1882	518	546	13			
1	C	372	Total	C	N	O	S	0	0	0
			3016	1918	530	555	13			
1	D	367	Total	C	N	O	S	0	0	0
			2963	1884	519	547	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ILE	-	expression tag	UNP P19490
A	-2	GLU	-	expression tag	UNP P19490
A	-1	GLU	-	expression tag	UNP P19490
A	0	ARG	-	expression tag	UNP P19490
A	1	GLY	-	expression tag	UNP P19490
A	2	ALA	-	expression tag	UNP P19490
A	3	MET	-	expression tag	UNP P19490
A	375	LEU	-	expression tag	UNP P19490
A	376	GLU	-	expression tag	UNP P19490
A	377	VAL	-	expression tag	UNP P19490
A	378	LEU	-	expression tag	UNP P19490
A	379	PHE	-	expression tag	UNP P19490
A	380	GLN	-	expression tag	UNP P19490
B	-3	ILE	-	expression tag	UNP P19490
B	-2	GLU	-	expression tag	UNP P19490
B	-1	GLU	-	expression tag	UNP P19490
B	0	ARG	-	expression tag	UNP P19490
B	1	GLY	-	expression tag	UNP P19490
B	2	ALA	-	expression tag	UNP P19490
B	3	MET	-	expression tag	UNP P19490
B	375	LEU	-	expression tag	UNP P19490

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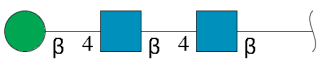
Chain	Residue	Modelled	Actual	Comment	Reference
B	376	GLU	-	expression tag	UNP P19490
B	377	VAL	-	expression tag	UNP P19490
B	378	LEU	-	expression tag	UNP P19490
B	379	PHE	-	expression tag	UNP P19490
B	380	GLN	-	expression tag	UNP P19490
C	-3	ILE	-	expression tag	UNP P19490
C	-2	GLU	-	expression tag	UNP P19490
C	-1	GLU	-	expression tag	UNP P19490
C	0	ARG	-	expression tag	UNP P19490
C	1	GLY	-	expression tag	UNP P19490
C	2	ALA	-	expression tag	UNP P19490
C	3	MET	-	expression tag	UNP P19490
C	375	LEU	-	expression tag	UNP P19490
C	376	GLU	-	expression tag	UNP P19490
C	377	VAL	-	expression tag	UNP P19490
C	378	LEU	-	expression tag	UNP P19490
C	379	PHE	-	expression tag	UNP P19490
C	380	GLN	-	expression tag	UNP P19490
D	-3	ILE	-	expression tag	UNP P19490
D	-2	GLU	-	expression tag	UNP P19490
D	-1	GLU	-	expression tag	UNP P19490
D	0	ARG	-	expression tag	UNP P19490
D	1	GLY	-	expression tag	UNP P19490
D	2	ALA	-	expression tag	UNP P19490
D	3	MET	-	expression tag	UNP P19490
D	375	LEU	-	expression tag	UNP P19490
D	376	GLU	-	expression tag	UNP P19490
D	377	VAL	-	expression tag	UNP P19490
D	378	LEU	-	expression tag	UNP P19490
D	379	PHE	-	expression tag	UNP P19490
D	380	GLN	-	expression tag	UNP P19490

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

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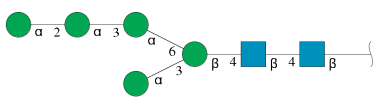
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	H	3	Total C N O 39 22 2 15	0	0	0
2	N	3	Total C N O 39 22 2 15	0	0	0

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

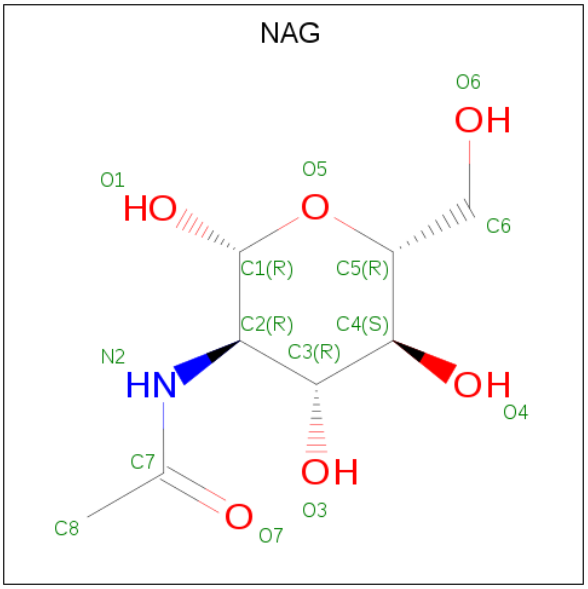
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	2	Total C N O 28 16 2 10	0	0	0
3	G	2	Total C N O 28 16 2 10	0	0	0
3	I	2	Total C N O 28 16 2 10	0	0	0
3	J	2	Total C N O 28 16 2 10	0	0	0
3	K	2	Total C N O 28 16 2 10	0	0	0
3	L	2	Total C N O 28 16 2 10	0	0	0
3	O	2	Total C N O 28 16 2 10	0	0	0
3	P	2	Total C N O 28 16 2 10	0	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	M	7	Total C N O 83 46 2 35	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

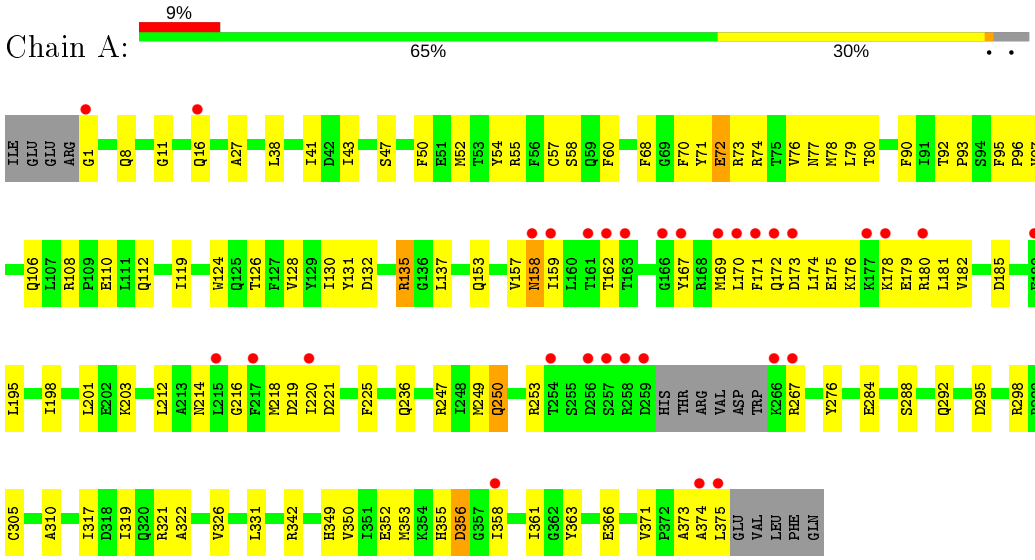
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	49	Total O 49 49	0	0
6	B	29	Total O 29 29	0	0
6	C	41	Total O 41 41	0	0
6	D	24	Total O 24 24	0	0

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.

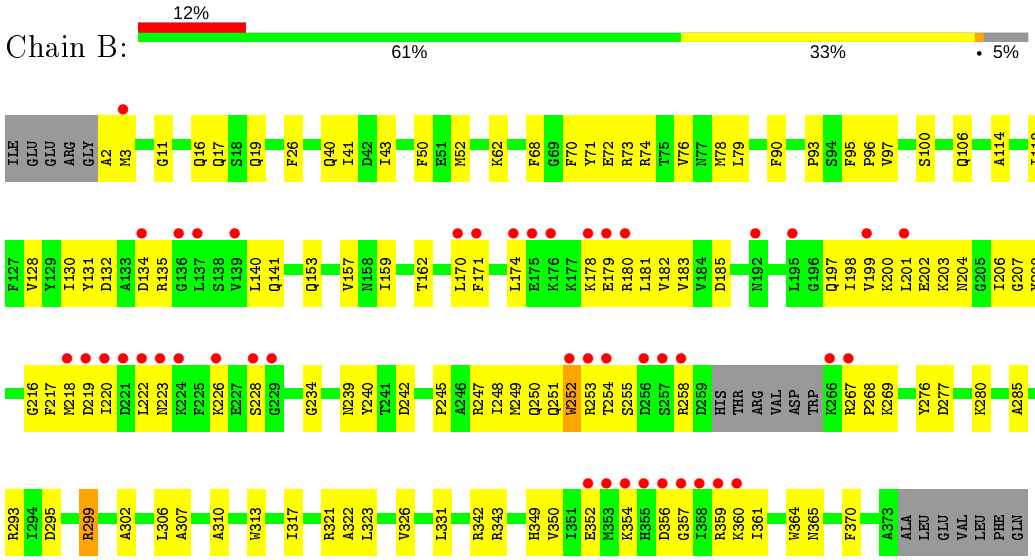
- Molecule 1: Glutamate receptor 1

Chain A:

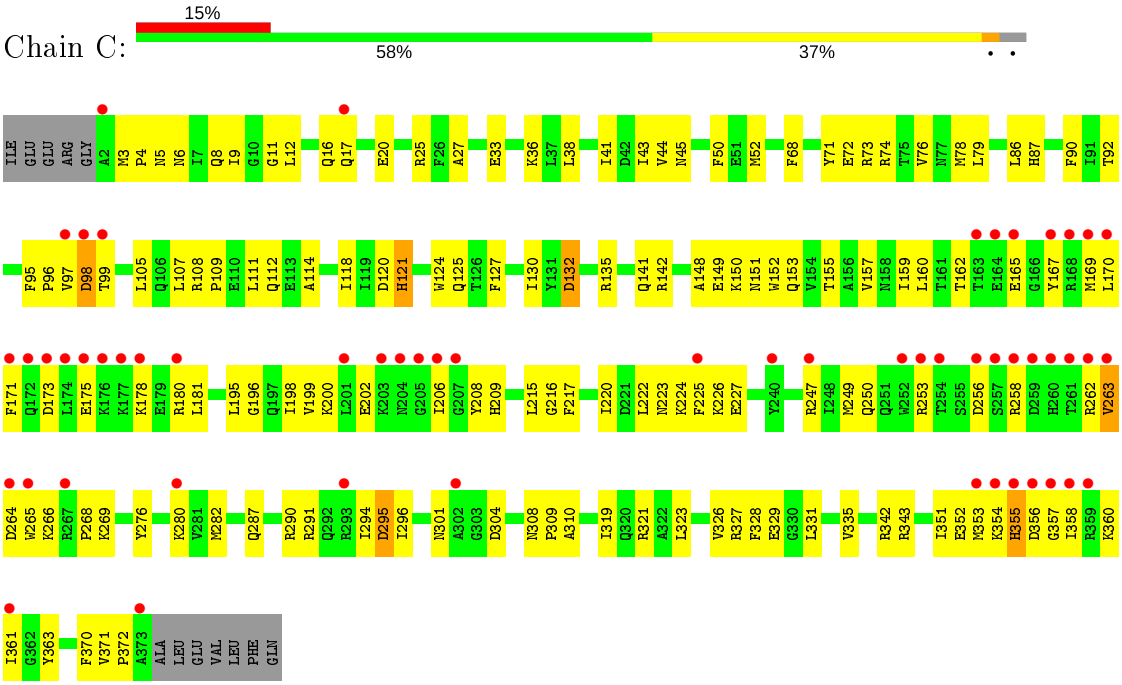


- Molecule 1: Glutamate receptor 1

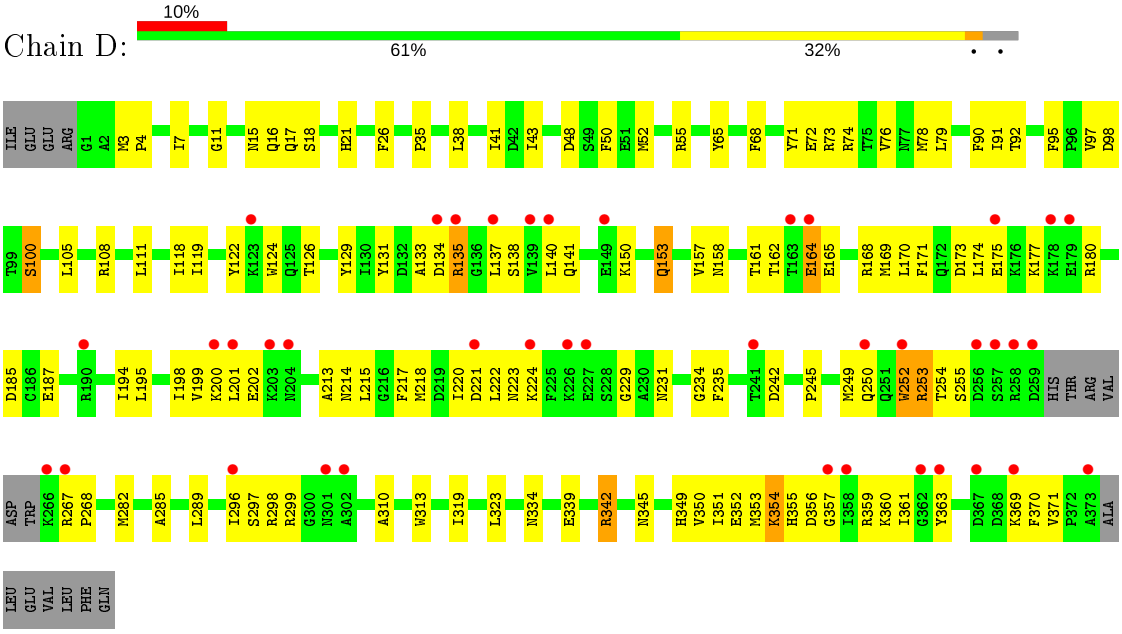
Chain B:



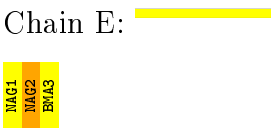
- Molecule 1: Glutamate receptor 1



• Molecule 1: Glutamate receptor 1

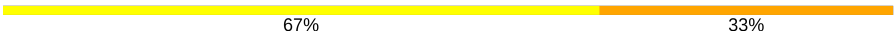


• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



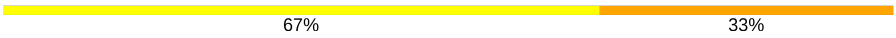
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain N:



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

Chain F:

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

Chain G:

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

Chain I:

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

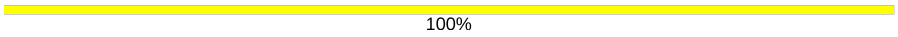
Chain J:

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

Chain K:

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

Chain L:

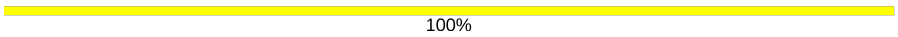


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

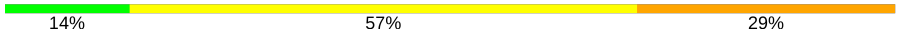
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

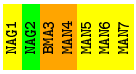
Chain P:



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

Chain M:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.59Å 94.42Å 186.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.18 – 2.50 41.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (93.18-2.50) 99.3 (41.46-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.66 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.218 , 0.286 0.234 , 0.278	Depositor DCC
R_{free} test set	2894 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	45.1	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12534	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.56	0/3049	0.66	1/4122 (0.0%)
1	B	0.50	0/3021	0.66	1/4085 (0.0%)
1	C	0.51	1/3082 (0.0%)	0.65	1/4171 (0.0%)
1	D	0.48	0/3025	0.65	2/4090 (0.0%)
All	All	0.52	1/12177 (0.0%)	0.65	5/16468 (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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	268	PRO	N-CD	5.01	1.54	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	294	ILE	N-CA-C	-5.44	96.32	111.00
1	D	342	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	158	ASN	N-CA-C	-5.34	96.58	111.00
1	D	100	SER	N-CA-C	-5.34	96.59	111.00
1	B	343	ARG	NE-CZ-NH2	-5.33	117.64	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	299	ARG	Sidechain

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	2987	0	2956	162	0
1	B	2959	0	2920	173	0
1	C	3016	0	2973	193	0
1	D	2963	0	2925	160	0
2	E	39	0	34	2	0
2	H	39	0	34	2	0
2	N	39	0	34	2	0
3	F	28	0	25	1	0
3	G	28	0	25	0	0
3	I	28	0	25	1	0
3	J	28	0	25	0	0
3	K	28	0	25	3	0
3	L	28	0	25	0	0
3	O	28	0	25	4	0
3	P	28	0	25	0	0
4	M	83	0	70	1	0
5	A	14	0	13	1	0
5	B	14	0	13	1	0
5	D	14	0	13	4	0
6	A	49	0	0	3	0
6	B	29	0	0	3	0
6	C	41	0	0	4	0
6	D	24	0	0	1	0
All	All	12534	0	12185	675	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 28.

All (675) 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:D:73:ARG:HB2	1:D:134:ASP:O	1.25	1.29
1:C:352:GLU:HB2	1:C:361:ILE:CD1	1.65	1.25
1:D:26:PHE:CZ	1:D:252:TRP:HB3	1.72	1.23
1:C:11:GLY:HA3	1:C:41:ILE:HG22	1.23	1.17
1:A:126:THR:HG22	1:A:153:GLN:HB2	1.22	1.17
1:D:133:ALA:HB2	1:D:158:ASN:HD21	1.09	1.17
1:C:226:LYS:HG2	1:C:356:ASP:OD1	1.44	1.16
1:C:352:GLU:CB	1:C:361:ILE:HD11	1.74	1.15
1:D:3:MET:HG2	1:D:4:PRO:CD	1.77	1.15
1:B:197:GLN:O	1:B:201:LEU:HG	1.47	1.15
1:B:203:LYS:HD2	1:B:208:TYR:CZ	1.81	1.15
1:B:349:HIS:HD2	1:B:360:LYS:HE2	1.11	1.14
1:C:44:VAL:HG11	1:C:52:MET:HE1	1.29	1.14
1:B:203:LYS:HD2	1:B:208:TYR:CE2	1.84	1.12
1:D:133:ALA:HB2	1:D:158:ASN:ND2	1.65	1.10
1:D:11:GLY:HA3	1:D:41:ILE:HG22	1.24	1.10
1:A:128:VAL:HG21	1:A:180:ARG:HH21	0.98	1.10
1:B:349:HIS:CD2	1:B:360:LYS:HE2	1.86	1.10
1:B:255:SER:HA	1:B:258:ARG:HD2	1.27	1.09
1:A:249:MET:O	1:A:253:ARG:HG2	1.53	1.07
1:B:76:VAL:HG21	1:B:97:VAL:HG11	1.34	1.06
1:A:174:LEU:HG	1:A:174:LEU:O	1.56	1.06
1:A:16:GLN:HB2	1:A:43:ILE:HD11	1.39	1.04
1:A:374:ALA:O	1:A:375:LEU:HD13	1.56	1.04
1:B:203:LYS:CD	1:B:208:TYR:CE2	2.41	1.04
1:B:216:GLY:O	1:B:219:ASP:HB2	1.56	1.03
1:C:353:MET:HE2	1:C:358:ILE:HD11	1.40	1.03
1:D:3:MET:CG	1:D:4:PRO:HD2	1.89	1.03
1:B:252:TRP:HA	1:B:255:SER:HB3	1.41	1.02
1:D:3:MET:HG2	1:D:4:PRO:HD2	1.02	1.01
1:D:133:ALA:CB	1:D:158:ASN:HD21	1.73	1.01
1:D:71:TYR:CD1	1:D:76:VAL:HG12	1.94	1.01
1:A:126:THR:CG2	1:A:153:GLN:HB2	1.91	1.00
1:B:249:MET:HB3	1:B:253:ARG:NH1	1.74	1.00
1:D:126:THR:HG22	1:D:153:GLN:HB3	1.44	1.00
1:B:132:ASP:HB2	6:B:406:HOH:O	1.61	0.99
1:C:96:PRO:HD3	1:C:108:ARG:HD2	1.41	0.99
1:C:9:ILE:HD12	1:C:282:MET:HE2	1.44	0.98
1:A:135:ARG:CG	1:A:135:ARG:HH11	1.76	0.98
1:B:349:HIS:CD2	1:B:360:LYS:CE	2.46	0.98
1:C:352:GLU:HB2	1:C:361:ILE:HD11	1.00	0.97
1:C:3:MET:SD	1:C:296:ILE:HD11	2.04	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:MET:HA	1:D:357:GLY:O	1.64	0.97
1:C:263:VAL:HG12	1:C:264:ASP:H	1.29	0.97
1:A:135:ARG:HG3	1:A:135:ARG:HH11	1.30	0.97
1:D:91:ILE:HD13	1:D:282:MET:HE3	1.43	0.96
1:C:352:GLU:OE2	1:C:354:LYS:HE3	1.64	0.95
1:A:128:VAL:HG21	1:A:180:ARG:NH2	1.80	0.95
1:B:249:MET:CB	1:B:253:ARG:NH1	2.30	0.95
1:C:353:MET:HE2	1:C:358:ILE:CD1	1.97	0.95
1:B:170:LEU:O	1:B:174:LEU:HG	1.66	0.95
1:C:199:VAL:O	1:C:202:GLU:HG2	1.67	0.94
1:B:157:VAL:HG13	1:B:162:THR:HG21	1.49	0.94
1:D:71:TYR:CE1	1:D:76:VAL:HG12	2.02	0.94
1:B:174:LEU:CD2	1:B:180:ARG:HD3	1.98	0.94
1:C:44:VAL:HG21	1:C:52:MET:HE3	1.46	0.94
1:A:131:TYR:CZ	1:A:158:ASN:HB2	2.03	0.93
1:B:349:HIS:HD2	1:B:360:LYS:CE	1.82	0.93
1:D:126:THR:HG22	1:D:153:GLN:CB	1.98	0.93
1:D:26:PHE:CE1	1:D:252:TRP:HB3	2.04	0.93
1:A:159:ILE:HD12	1:A:167:TYR:OH	1.70	0.92
1:B:174:LEU:HD23	1:B:180:ARG:HD3	1.52	0.91
1:B:203:LYS:HD2	1:B:208:TYR:OH	1.68	0.91
1:C:165:GLU:O	1:C:169:MET:HG2	1.68	0.91
1:A:374:ALA:O	1:A:375:LEU:CD1	2.19	0.90
1:B:26:PHE:CE1	1:B:252:TRP:HB3	2.06	0.90
1:D:91:ILE:HD13	1:D:282:MET:CE	2.01	0.90
1:D:3:MET:CG	1:D:4:PRO:CD	2.47	0.89
1:A:1:GLY:N	1:A:295:ASP:HB2	1.87	0.89
1:A:190:ARG:HG2	1:A:194:ILE:HD12	1.54	0.88
1:C:181:LEU:HD23	1:C:209:HIS:HB2	1.55	0.88
1:D:135:ARG:HG3	1:D:135:ARG:HH11	1.35	0.88
1:A:169:MET:SD	1:A:169:MET:O	2.32	0.88
1:A:99:THR:HG22	1:A:99:THR:O	1.71	0.88
1:C:130:ILE:HD11	1:C:167:TYR:HE1	1.39	0.88
1:A:170:LEU:HD12	1:A:180:ARG:HH22	1.39	0.87
1:B:350:VAL:O	1:B:361:ILE:HG22	1.73	0.87
1:C:353:MET:CE	1:C:358:ILE:CD1	2.51	0.87
1:A:170:LEU:CD1	1:A:180:ARG:HH22	1.88	0.87
1:B:106:GLN:NE2	1:B:342:ARG:HD3	1.90	0.86
1:A:57:CYS:HG	1:A:305:CYS:HG	1.07	0.86
1:B:216:GLY:HA3	1:B:219:ASP:OD2	1.75	0.86
1:A:175:GLU:O	1:A:176:LYS:HB2	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:ARG:CG	1:D:135:ARG:HH11	1.90	0.85
1:A:131:TYR:O	1:A:158:ASN:HA	1.76	0.85
1:A:353:MET:HB2	1:A:358:ILE:HG22	1.59	0.85
1:C:99:THR:HG22	1:C:99:THR:O	1.77	0.84
1:A:195:LEU:HD23	1:A:225:PHE:CE2	2.12	0.84
1:B:204:ASN:O	1:B:228:SER:HB3	1.78	0.84
1:C:181:LEU:CD2	1:C:209:HIS:HB2	2.07	0.84
1:D:95:PHE:CD2	1:D:135:ARG:HB2	2.11	0.84
1:B:239:ASN:HB3	1:B:242:ASP:OD2	1.77	0.84
1:B:249:MET:HB2	1:B:253:ARG:HH12	1.41	0.84
1:A:220:ILE:HG22	1:A:221:ASP:N	1.93	0.83
1:A:363:TYR:CZ	1:A:371:VAL:HG21	2.13	0.83
1:A:159:ILE:HG23	1:A:167:TYR:OH	1.77	0.83
1:A:352:GLU:OE1	1:A:361:ILE:HG21	1.79	0.83
1:A:11:GLY:HA2	1:A:68:PHE:O	1.80	0.82
1:D:65:TYR:HE1	1:D:296:ILE:HG22	1.43	0.82
1:C:217:PHE:O	1:C:220:ILE:HG12	1.79	0.82
1:A:97:VAL:HG12	1:A:98:ASP:N	1.95	0.82
1:A:236:GLN:OE1	1:A:267:ARG:NH2	2.13	0.81
1:C:263:VAL:HG12	1:C:264:ASP:N	1.95	0.81
1:C:124:TRP:CD1	1:C:181:LEU:HD13	2.16	0.81
1:B:249:MET:CB	1:B:253:ARG:HH12	1.92	0.80
1:D:296:ILE:HD13	1:D:319:ILE:HD11	1.63	0.80
1:C:226:LYS:CG	1:C:356:ASP:OD1	2.29	0.80
1:C:223:ASN:O	1:C:227:GLU:HG3	1.81	0.80
1:A:71:TYR:CE2	1:A:92:THR:HG21	2.17	0.80
1:B:128:VAL:HG21	1:B:174:LEU:HD21	1.64	0.80
1:B:203:LYS:CD	1:B:208:TYR:HE2	1.95	0.80
1:D:11:GLY:CA	1:D:41:ILE:HG22	2.09	0.80
1:B:285:ALA:CB	1:B:323:LEU:HD23	2.12	0.79
1:C:124:TRP:CG	1:C:181:LEU:HD13	2.16	0.79
1:A:374:ALA:O	1:A:375:LEU:HB2	1.82	0.79
1:C:352:GLU:CG	1:C:361:ILE:HD11	2.12	0.79
1:D:363:TYR:CZ	1:D:371:VAL:HG21	2.18	0.79
1:B:40:GLN:OE1	1:B:62:LYS:HD3	1.82	0.79
1:A:191:LEU:HD21	1:A:212:LEU:HD13	1.64	0.79
1:D:73:ARG:CB	1:D:134:ASP:O	2.20	0.78
1:C:121:HIS:C	1:C:121:HIS:ND1	2.36	0.78
1:C:171:PHE:CD1	1:C:180:ARG:HD3	2.19	0.78
1:A:135:ARG:NH1	1:A:135:ARG:HG3	1.97	0.78
1:B:124:TRP:CZ2	1:B:181:LEU:HB3	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LYS:HD3	1:B:208:TYR:CE2	2.18	0.78
1:D:26:PHE:CE2	1:D:252:TRP:HB3	2.19	0.78
1:C:71:TYR:HD2	1:C:90:PHE:HE2	1.30	0.77
1:A:220:ILE:HG22	1:A:221:ASP:H	1.45	0.77
1:D:133:ALA:HB2	1:D:158:ASN:CG	2.04	0.77
1:C:72:GLU:HG2	1:C:73:ARG:H	1.48	0.77
1:C:372:PRO:HB2	6:C:408:HOH:O	1.83	0.77
1:C:363:TYR:CZ	1:C:371:VAL:HG21	2.20	0.77
1:A:342:ARG:HH11	1:A:342:ARG:HG3	1.50	0.76
1:B:220:ILE:HG22	1:B:220:ILE:O	1.84	0.76
1:A:50:PHE:CE2	1:C:310:ALA:HB2	2.21	0.76
1:C:132:ASP:OD1	1:C:159:ILE:HD11	1.85	0.76
1:B:285:ALA:HB2	1:B:323:LEU:HD23	1.66	0.76
1:A:220:ILE:CG2	1:A:221:ASP:H	1.99	0.76
1:C:44:VAL:HG11	1:C:52:MET:CE	2.13	0.75
1:D:296:ILE:CD1	1:D:319:ILE:HD11	2.16	0.75
1:A:126:THR:HG22	1:A:153:GLN:CB	2.09	0.75
1:B:203:LYS:HD3	1:B:208:TYR:HE2	1.51	0.75
1:C:71:TYR:HD2	1:C:90:PHE:CE2	2.04	0.75
1:B:50:PHE:CE2	1:D:310:ALA:HB2	2.22	0.75
1:B:247:ARG:O	1:B:251:GLN:HG3	1.87	0.75
1:A:172:GLN:OE1	1:C:151:ASN:HB2	1.87	0.75
5:A:900:NAG:O6	6:A:417:HOH:O	2.04	0.75
1:B:249:MET:HB3	1:B:253:ARG:HH11	1.51	0.75
1:D:71:TYR:HD2	1:D:90:PHE:HE2	1.35	0.75
1:B:131:TYR:OH	1:D:141:GLN:NE2	2.20	0.74
1:D:360:LYS:HD2	5:D:900:NAG:O3	1.87	0.74
1:C:71:TYR:CD2	1:C:90:PHE:HE2	2.04	0.74
1:B:220:ILE:CG2	1:B:220:ILE:O	2.36	0.74
1:C:155:THR:OG1	1:C:170:LEU:HD21	1.88	0.74
1:C:178:LYS:O	1:C:206:ILE:HG13	1.86	0.74
1:C:44:VAL:CG2	1:C:52:MET:HE3	2.18	0.74
1:A:373:ALA:O	1:A:375:LEU:HD12	1.88	0.73
1:A:71:TYR:HE2	1:A:92:THR:HG21	1.51	0.73
1:D:11:GLY:HA3	1:D:41:ILE:CG2	2.10	0.73
1:B:302:ALA:HB3	1:C:5:ASN:HB3	1.70	0.73
1:C:352:GLU:HB2	1:C:361:ILE:CG1	2.17	0.73
1:D:135:ARG:NH1	1:D:185:ASP:OD2	2.20	0.73
1:A:170:LEU:CD1	1:A:180:ARG:NH2	2.51	0.73
1:A:1:GLY:H3	1:A:295:ASP:HB2	1.51	0.73
1:A:352:GLU:HB2	1:A:361:ILE:HD13	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:VAL:CG1	1:C:52:MET:HE1	2.14	0.73
1:C:124:TRP:HZ2	1:C:209:HIS:HB3	1.53	0.73
1:C:4:PRO:HD2	1:C:296:ILE:CD1	2.19	0.72
1:D:218:MET:O	1:D:267:ARG:NH2	2.22	0.72
1:A:71:TYR:HD2	1:A:90:PHE:HE2	1.37	0.72
1:C:199:VAL:HA	1:C:202:GLU:OE2	1.88	0.72
1:C:11:GLY:CA	1:C:41:ILE:HG22	2.13	0.72
1:C:353:MET:HE3	1:C:358:ILE:HD12	1.72	0.72
1:B:141:GLN:NE2	1:D:131:TYR:OH	2.22	0.72
1:D:65:TYR:HE1	1:D:296:ILE:CG2	2.03	0.72
1:B:248:ILE:HG21	1:B:331:LEU:HD21	1.72	0.72
1:B:242:ASP:HB2	1:B:245:PRO:HG2	1.70	0.71
1:C:71:TYR:CE2	1:C:92:THR:HG21	2.25	0.71
1:C:124:TRP:CZ2	1:C:181:LEU:HD22	2.26	0.71
1:C:353:MET:CE	1:C:358:ILE:HD12	2.20	0.71
1:B:130:ILE:HG22	1:B:159:ILE:HD11	1.71	0.71
1:B:217:PHE:CD1	1:B:234:GLY:HA3	2.25	0.71
1:D:168:ARG:HD2	1:D:201:LEU:HD11	1.72	0.71
1:A:1:GLY:H2	1:A:295:ASP:HB2	1.56	0.71
1:D:352:GLU:OE2	3:O:1:NAG:C1	2.39	0.70
1:D:71:TYR:CD2	1:D:90:PHE:HE2	2.09	0.70
1:A:130:ILE:CG2	1:A:159:ILE:HD11	2.20	0.70
1:D:285:ALA:HB2	1:D:323:LEU:HD23	1.72	0.70
1:C:124:TRP:CE2	1:C:181:LEU:HD22	2.26	0.70
1:B:171:PHE:CD1	1:B:174:LEU:HD12	2.26	0.70
1:C:52:MET:HB3	1:C:78:MET:HE1	1.73	0.69
1:A:171:PHE:CZ	1:A:203:LYS:HE2	2.27	0.69
1:C:124:TRP:CZ3	1:C:181:LEU:HB3	2.27	0.69
1:C:130:ILE:HD11	1:C:167:TYR:CE1	2.26	0.69
1:B:70:PHE:CE1	1:B:93:PRO:HG2	2.27	0.69
1:A:310:ALA:HB2	1:C:50:PHE:CE2	2.28	0.69
1:A:124:TRP:CG	1:A:181:LEU:HD13	2.27	0.68
1:B:354:LYS:O	1:B:357:GLY:N	2.26	0.68
1:D:71:TYR:HD2	1:D:90:PHE:CE2	2.11	0.68
1:A:97:VAL:HG12	1:A:98:ASP:H	1.57	0.68
1:B:174:LEU:HD22	1:B:180:ARG:HD3	1.74	0.68
1:B:307:ALA:HB2	1:C:38:LEU:HD12	1.75	0.68
1:C:263:VAL:CG1	1:C:264:ASP:H	2.05	0.68
1:D:105:LEU:CD1	1:D:323:LEU:HB3	2.24	0.68
1:C:253:ARG:NH2	1:C:266:LYS:O	2.27	0.68
1:B:52:MET:CE	1:B:79:LEU:HD11	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ALA:O	1:A:375:LEU:CB	2.42	0.68
1:A:95:PHE:CD2	1:A:135:ARG:O	2.47	0.67
1:B:11:GLY:HA3	1:B:41:ILE:HG22	1.76	0.67
1:A:167:TYR:HB2	1:A:201:LEU:HD13	1.75	0.67
1:D:164:GLU:CD	1:D:164:GLU:H	1.96	0.67
1:C:8:GLN:HG3	1:C:38:LEU:HD23	1.76	0.67
1:A:11:GLY:HA3	1:A:41:ILE:HG22	1.77	0.67
1:D:126:THR:HG22	1:D:153:GLN:HB2	1.77	0.67
1:B:179:GLU:HB2	1:B:207:GLY:O	1.95	0.66
1:B:26:PHE:CZ	1:B:252:TRP:HB3	2.29	0.66
1:A:52:MET:HB2	1:A:78:MET:HE1	1.77	0.66
1:A:80:THR:O	1:A:101:ASN:ND2	2.27	0.66
1:B:299:ARG:HD2	1:B:313:TRP:CE2	2.30	0.66
1:C:11:GLY:HA2	1:C:68:PHE:O	1.95	0.66
1:C:352:GLU:OE2	1:C:354:LYS:CE	2.42	0.66
1:B:130:ILE:CG2	1:B:159:ILE:HD11	2.26	0.66
1:C:124:TRP:CH2	1:C:181:LEU:HB3	2.31	0.66
1:C:4:PRO:HD2	1:C:296:ILE:HD12	1.78	0.66
1:C:74:ARG:NH1	3:K:2:NAG:O7	2.28	0.66
1:A:363:TYR:CZ	1:A:371:VAL:CG2	2.79	0.66
1:D:165:GLU:O	1:D:169:MET:HG2	1.95	0.65
1:B:321:ARG:HG2	1:C:258:ARG:NE	2.11	0.65
1:C:175:GLU:OE2	1:C:178:LYS:NZ	2.27	0.65
1:C:180:ARG:NE	1:C:206:ILE:HD13	2.12	0.65
1:D:289:LEU:HD13	1:D:296:ILE:HD11	1.78	0.65
1:D:17:GLN:HE22	3:K:1:NAG:H81	1.61	0.65
1:A:130:ILE:HG23	1:A:159:ILE:HD11	1.78	0.65
1:D:72:GLU:OE2	1:D:74:ARG:HD3	1.97	0.64
1:C:180:ARG:CD	1:C:206:ILE:HD13	2.28	0.64
1:B:310:ALA:HB2	1:D:50:PHE:CE2	2.32	0.64
1:A:130:ILE:HG23	1:A:159:ILE:CG1	2.27	0.64
1:A:130:ILE:HG23	1:A:159:ILE:HG12	1.78	0.64
1:A:374:ALA:C	1:A:375:LEU:CD1	2.65	0.64
1:B:254:THR:O	1:B:258:ARG:HG3	1.97	0.64
1:C:71:TYR:HE2	1:C:92:THR:HG21	1.61	0.64
1:D:71:TYR:CD1	1:D:76:VAL:CG1	2.78	0.64
1:A:71:TYR:CB	1:A:79:LEU:HD12	2.28	0.64
1:A:97:VAL:CG1	1:A:98:ASP:N	2.60	0.64
1:C:44:VAL:HG21	1:C:52:MET:CE	2.26	0.64
1:A:52:MET:CB	1:A:78:MET:HE1	2.28	0.64
1:B:216:GLY:O	1:B:219:ASP:CB	2.42	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:ARG:HG3	1:D:135:ARG:NH1	2.08	0.64
1:B:74:ARG:HH21	2:H:2:NAG:H83	1.63	0.63
1:C:353:MET:HE3	1:C:358:ILE:CD1	2.26	0.63
1:A:130:ILE:HG23	1:A:159:ILE:CD1	2.28	0.63
1:A:95:PHE:CE2	1:A:135:ARG:O	2.51	0.63
1:A:74:ARG:NH1	2:E:2:NAG:H83	2.13	0.63
1:B:132:ASP:OD1	1:B:135:ARG:NH2	2.32	0.63
1:B:72:GLU:CD	1:B:73:ARG:N	2.51	0.63
1:B:52:MET:CB	1:B:78:MET:HE2	2.29	0.63
1:C:178:LYS:O	1:C:206:ILE:CG1	2.46	0.63
1:A:159:ILE:CD1	1:A:167:TYR:OH	2.44	0.63
1:A:97:VAL:CG1	1:A:98:ASP:H	2.11	0.63
1:C:351:ILE:CD1	1:C:360:LYS:HG3	2.29	0.63
1:D:133:ALA:HB2	1:D:158:ASN:OD1	1.99	0.63
1:D:73:ARG:HD3	1:D:137:LEU:HD23	1.81	0.62
1:D:352:GLU:OE2	3:O:1:NAG:N2	2.30	0.62
1:D:15:ASN:O	1:D:21:HIS:NE2	2.31	0.62
1:B:157:VAL:CG1	1:B:162:THR:HG21	2.25	0.62
1:C:301:ASN:O	1:C:304:ASP:HB2	2.00	0.62
1:D:52:MET:HB3	1:D:78:MET:CE	2.28	0.62
1:A:124:TRP:CD1	1:A:181:LEU:HD13	2.34	0.62
1:C:363:TYR:CZ	1:C:371:VAL:CG2	2.83	0.62
1:B:52:MET:HB3	1:B:78:MET:HE2	1.82	0.62
1:C:226:LYS:HE2	1:C:356:ASP:CG	2.20	0.62
1:A:135:ARG:HH21	1:A:214:ASN:HB2	1.64	0.62
1:A:71:TYR:HB3	1:A:79:LEU:CD1	2.30	0.62
1:B:307:ALA:HB2	1:C:38:LEU:CD1	2.30	0.62
1:A:131:TYR:CE1	1:A:158:ASN:HB2	2.34	0.62
1:D:17:GLN:NE2	3:K:1:NAG:H81	2.15	0.62
1:A:249:MET:O	1:A:253:ARG:CG	2.42	0.62
1:C:199:VAL:O	1:C:202:GLU:CG	2.45	0.62
1:A:170:LEU:HD12	1:A:180:ARG:NH2	2.12	0.62
1:B:354:LYS:HB2	3:I:1:NAG:O7	2.00	0.61
1:B:40:GLN:HE22	1:B:62:LYS:HE2	1.63	0.61
1:C:196:GLY:O	1:C:200:LYS:HE3	2.00	0.61
1:B:248:ILE:CG2	1:B:331:LEU:HD21	2.31	0.61
1:A:170:LEU:HD13	1:A:180:ARG:NH2	2.14	0.61
1:A:353:MET:CB	1:A:358:ILE:HG22	2.29	0.61
1:C:16:GLN:HG3	1:C:43:ILE:HD11	1.82	0.61
1:D:249:MET:HE2	1:D:268:PRO:CD	2.31	0.61
1:B:52:MET:HB3	1:B:78:MET:CE	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLU:HG2	1:A:73:ARG:H	1.65	0.60
1:B:106:GLN:HE21	1:B:342:ARG:HD3	1.65	0.60
1:C:52:MET:HA	1:C:52:MET:CE	2.30	0.60
1:B:239:ASN:HB3	1:B:242:ASP:CG	2.20	0.60
1:B:197:GLN:O	1:B:201:LEU:CG	2.37	0.60
1:D:371:VAL:O	1:D:371:VAL:CG2	2.48	0.60
1:B:95:PHE:CD1	1:B:96:PRO:HD2	2.37	0.59
1:C:352:GLU:CD	1:C:361:ILE:HD11	2.22	0.59
1:C:52:MET:HE2	1:C:52:MET:HA	1.82	0.59
1:C:72:GLU:HG2	1:C:73:ARG:N	2.17	0.59
1:A:132:ASP:C	1:A:132:ASP:OD1	2.40	0.59
1:B:71:TYR:HD2	1:B:90:PHE:HE2	1.50	0.59
1:C:206:ILE:HG23	1:C:208:TYR:CE1	2.37	0.59
1:C:195:LEU:HB3	1:C:225:PHE:CZ	2.36	0.59
1:D:65:TYR:CE1	1:D:296:ILE:CG2	2.84	0.59
1:D:11:GLY:HA2	1:D:68:PHE:O	2.02	0.59
1:A:191:LEU:HD23	1:A:220:ILE:HG13	1.85	0.59
1:C:76:VAL:HG21	1:C:97:VAL:HG11	1.84	0.59
1:D:111:LEU:HD13	1:D:215:LEU:HD21	1.83	0.59
1:D:352:GLU:HB2	1:D:361:ILE:HD11	1.84	0.59
1:A:288:SER:O	1:A:292:GLN:HB2	2.03	0.59
1:B:114:ALA:O	1:B:118:ILE:HG12	2.03	0.59
1:B:124:TRP:CD1	1:B:181:LEU:HD13	2.37	0.59
1:A:52:MET:CE	1:A:79:LEU:HD11	2.33	0.59
1:C:157:VAL:HG13	1:C:162:THR:OG1	2.03	0.59
1:C:124:TRP:CE3	1:C:181:LEU:HB3	2.38	0.59
1:B:72:GLU:CD	1:B:73:ARG:H	2.06	0.58
1:C:52:MET:HB3	1:C:78:MET:CE	2.32	0.58
1:A:52:MET:HB2	1:A:78:MET:CE	2.33	0.58
1:A:157:VAL:HG13	1:A:162:THR:HG21	1.85	0.58
1:C:249:MET:CE	1:C:331:LEU:HD11	2.33	0.58
1:C:159:ILE:HG13	1:C:160:LEU:HG	1.84	0.58
1:A:247:ARG:O	1:A:250:GLN:HB3	2.03	0.58
1:B:128:VAL:CG2	1:B:174:LEU:HD21	2.33	0.58
1:D:16:GLN:HG3	1:D:43:ILE:CD1	2.33	0.58
1:B:242:ASP:OD1	5:B:900:NAG:O5	2.22	0.58
1:A:342:ARG:NH1	1:A:342:ARG:HG3	2.16	0.58
1:C:111:LEU:HD21	1:C:215:LEU:HG	1.86	0.58
1:C:6:ASN:HD22	1:C:36:LYS:HB3	1.69	0.58
1:A:110:GLU:CD	1:A:112:GLN:HE22	2.08	0.57
1:C:263:VAL:O	1:C:264:ASP:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:PRO:HD3	1:A:108:ARG:HD2	1.86	0.57
1:A:374:ALA:C	1:A:375:LEU:HD12	2.24	0.57
1:B:17:GLN:HG3	1:B:17:GLN:O	2.04	0.57
1:C:223:ASN:O	1:C:227:GLU:CG	2.52	0.57
1:D:16:GLN:HA	1:D:43:ILE:HD11	1.85	0.57
1:B:200:LYS:C	1:B:202:GLU:H	2.04	0.57
1:C:25:ARG:NH2	1:C:262:ARG:NH1	2.52	0.57
1:C:11:GLY:HA3	1:C:41:ILE:CG2	2.15	0.57
1:C:180:ARG:HG3	1:C:206:ILE:HD11	1.87	0.57
1:D:129:TYR:CE2	1:D:131:TYR:HB3	2.40	0.56
1:A:157:VAL:CG1	1:A:162:THR:HG21	2.35	0.56
1:C:17:GLN:NE2	2:N:1:NAG:H81	2.20	0.56
1:D:252:TRP:HA	1:D:255:SER:HB2	1.87	0.56
1:C:71:TYR:HB3	1:C:79:LEU:CD1	2.35	0.56
1:B:199:VAL:HG12	1:B:204:ASN:HD22	1.70	0.56
1:C:352:GLU:CD	1:C:354:LYS:HE3	2.25	0.56
1:A:218:MET:HG2	1:A:236:GLN:NE2	2.21	0.56
1:A:363:TYR:CE2	1:A:371:VAL:CG2	2.88	0.56
1:C:112:GLN:HG3	1:C:142:ARG:HG2	1.88	0.56
1:C:321:ARG:CZ	6:C:411:HOH:O	2.53	0.56
1:A:71:TYR:HD2	1:A:90:PHE:CE2	2.21	0.55
1:B:302:ALA:CB	1:C:5:ASN:HB3	2.35	0.55
1:A:52:MET:CB	1:A:78:MET:CE	2.85	0.55
1:B:171:PHE:CD2	1:B:201:LEU:HD13	2.41	0.55
1:C:124:TRP:CD2	1:C:181:LEU:HD13	2.41	0.55
1:D:194:ILE:HG22	1:D:198:ILE:HD12	1.89	0.55
1:B:217:PHE:C	1:B:219:ASP:H	2.09	0.55
1:B:95:PHE:CD2	1:B:134:ASP:HB3	2.41	0.55
1:C:180:ARG:NE	1:C:206:ILE:CD1	2.69	0.55
1:D:249:MET:HE2	1:D:268:PRO:HD2	1.88	0.55
1:D:363:TYR:CZ	1:D:371:VAL:CG2	2.90	0.55
1:A:220:ILE:CG2	1:A:221:ASP:N	2.56	0.55
1:B:17:GLN:O	1:B:17:GLN:CG	2.55	0.55
1:D:351:ILE:HD11	5:D:900:NAG:H81	1.87	0.55
1:A:178:LYS:C	1:A:179:GLU:HG2	2.26	0.55
1:B:131:TYR:CZ	1:B:140:LEU:HD22	2.42	0.55
1:B:306:LEU:O	6:B:391:HOH:O	2.18	0.55
1:B:40:GLN:OE1	1:B:62:LYS:CD	2.54	0.55
1:D:285:ALA:CB	1:D:323:LEU:HD23	2.36	0.55
1:C:16:GLN:HG3	1:C:43:ILE:CD1	2.37	0.55
1:B:293:ARG:HA	6:B:402:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:MET:CE	1:D:268:PRO:CD	2.85	0.54
1:C:321:ARG:NH2	6:C:411:HOH:O	2.39	0.54
1:B:52:MET:HE1	1:B:79:LEU:HD11	1.88	0.54
1:A:71:TYR:HB3	1:A:79:LEU:HD12	1.90	0.54
1:C:98:ASP:HA	1:C:342:ARG:NH2	2.23	0.54
1:D:71:TYR:CE1	1:D:76:VAL:CG1	2.86	0.54
1:B:350:VAL:C	1:B:361:ILE:HG22	2.27	0.54
1:B:130:ILE:CG2	1:B:159:ILE:CD1	2.85	0.54
1:B:277:ASP:OD1	1:B:280:LYS:NZ	2.40	0.53
1:B:185:ASP:HA	1:B:213:ALA:HB3	1.90	0.53
1:D:71:TYR:CE2	1:D:92:THR:HG21	2.43	0.53
1:C:52:MET:CB	1:C:78:MET:CE	2.86	0.53
3:F:1:NAG:H61	3:F:2:NAG:C7	2.38	0.53
1:A:27:ALA:HB2	1:A:276:TYR:CD1	2.43	0.53
1:A:71:TYR:HB2	1:A:79:LEU:HD12	1.88	0.53
1:A:99:THR:CG2	1:A:99:THR:O	2.45	0.53
1:A:135:ARG:HG2	1:A:135:ARG:HH11	1.69	0.53
1:B:124:TRP:CE2	1:B:181:LEU:HB3	2.43	0.53
1:C:99:THR:CG2	1:C:99:THR:O	2.50	0.53
1:B:19:GLN:OE1	1:B:269:LYS:HE3	2.09	0.53
1:D:371:VAL:O	1:D:371:VAL:HG23	2.09	0.53
1:B:74:ARG:NH2	2:H:2:NAG:H83	2.23	0.53
1:A:363:TYR:CE2	1:A:371:VAL:HG21	2.43	0.52
1:D:174:LEU:HD23	1:D:177:LYS:NZ	2.24	0.52
1:A:322:ALA:O	6:A:409:HOH:O	2.19	0.52
1:B:252:TRP:HD1	1:B:252:TRP:H	1.57	0.52
1:B:288:SER:O	1:B:292:GLN:HG3	2.09	0.52
1:B:349:HIS:CD2	1:B:360:LYS:HE3	2.42	0.52
1:D:195:LEU:HD11	1:D:220:ILE:CG2	2.39	0.52
1:D:214:ASN:O	1:D:235:PHE:HB2	2.10	0.52
1:D:361:ILE:CG2	1:D:370:PHE:HZ	2.22	0.52
1:B:179:GLU:HG3	1:B:207:GLY:HA3	1.92	0.52
1:D:98:ASP:O	1:D:342:ARG:NH2	2.43	0.52
1:C:125:GLN:O	1:C:152:TRP:HA	2.10	0.52
1:A:153:GLN:OE1	1:C:153:GLN:HG3	2.10	0.52
1:D:185:ASP:HA	1:D:213:ALA:HB3	1.92	0.52
1:B:52:MET:HE3	1:B:79:LEU:HD11	1.90	0.51
1:C:114:ALA:O	1:C:118:ILE:HG12	2.10	0.51
1:A:153:GLN:OE1	1:C:153:GLN:CG	2.58	0.51
1:B:171:PHE:HA	1:B:174:LEU:HD12	1.91	0.51
1:C:256:ASP:HB3	1:C:265:TRP:NE1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:GLN:HG3	1:D:43:ILE:HD11	1.91	0.51
1:C:253:ARG:HH22	1:C:266:LYS:C	2.13	0.51
1:D:3:MET:CG	1:D:4:PRO:HD3	2.39	0.51
1:B:201:LEU:O	1:B:203:LYS:HG2	2.10	0.51
1:C:124:TRP:CZ2	1:C:209:HIS:HB3	2.41	0.51
1:B:364:TRP:HD1	1:B:370:PHE:HB2	1.76	0.51
1:A:47:SER:OG	1:A:72:GLU:OE1	2.25	0.51
1:C:124:TRP:CZ2	1:C:181:LEU:HB3	2.45	0.51
1:C:95:PHE:CE1	1:C:135:ARG:NH2	2.79	0.51
1:D:126:THR:CG2	1:D:153:GLN:HB3	2.31	0.51
1:B:249:MET:HB2	1:B:253:ARG:NH1	2.07	0.51
1:C:249:MET:HE2	1:C:331:LEU:HD11	1.92	0.51
1:C:295:ASP:O	1:C:296:ILE:HG23	2.11	0.51
1:D:72:GLU:O	1:D:76:VAL:HG13	2.11	0.50
1:D:52:MET:CB	1:D:78:MET:CE	2.88	0.50
1:B:204:ASN:O	1:B:204:ASN:OD1	2.30	0.50
1:B:16:GLN:HA	1:B:43:ILE:CD1	2.41	0.50
1:D:352:GLU:HB2	1:D:361:ILE:CD1	2.41	0.50
1:A:236:GLN:HB3	1:A:349:HIS:HB2	1.93	0.50
1:B:40:GLN:NE2	1:B:62:LYS:HE2	2.27	0.50
1:A:169:MET:SD	1:A:169:MET:C	2.89	0.50
1:A:128:VAL:HB	1:A:182:VAL:HG22	1.93	0.50
1:D:252:TRP:HA	1:D:255:SER:CB	2.41	0.50
1:B:200:LYS:C	1:B:202:GLU:N	2.64	0.50
1:D:79:LEU:HD23	1:D:90:PHE:CE2	2.46	0.50
1:A:71:TYR:CD1	1:A:71:TYR:O	2.65	0.50
1:B:255:SER:O	1:B:258:ARG:HB2	2.11	0.50
1:D:363:TYR:CE2	1:D:371:VAL:HG21	2.47	0.50
1:A:132:ASP:OD1	1:A:132:ASP:O	2.30	0.50
1:D:352:GLU:OE2	3:O:1:NAG:C2	2.60	0.50
1:B:97:VAL:CG2	1:B:100:SER:HB3	2.41	0.49
1:D:108:ARG:NH1	1:D:187:GLU:OE2	2.39	0.49
1:D:296:ILE:HG22	1:D:297:SER:N	2.26	0.49
1:C:226:LYS:HE2	1:C:356:ASP:OD1	2.12	0.49
1:A:218:MET:CG	1:A:236:GLN:NE2	2.76	0.49
1:B:240:TYR:HD1	1:B:249:MET:HE2	1.78	0.49
1:D:171:PHE:O	1:D:175:GLU:HG2	2.12	0.49
1:D:352:GLU:O	1:D:357:GLY:O	2.30	0.49
1:B:239:ASN:CB	1:B:242:ASP:OD2	2.53	0.49
1:B:276:TYR:CE2	1:B:280:LYS:HD2	2.47	0.49
1:C:296:ILE:HG21	1:C:319:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:ARG:HA	1:D:201:LEU:HD21	1.94	0.49
1:D:105:LEU:HD13	1:D:323:LEU:HB3	1.95	0.49
1:D:356:ASP:OD1	1:D:356:ASP:O	2.30	0.49
1:B:130:ILE:HG22	1:B:159:ILE:CD1	2.40	0.49
1:B:72:GLU:CG	1:B:73:ARG:H	2.25	0.49
1:C:121:HIS:CD2	1:C:370:PHE:CE2	2.99	0.49
1:A:131:TYR:HA	1:A:185:ASP:O	2.13	0.49
1:D:242:ASP:HB3	1:D:245:PRO:HG2	1.93	0.49
1:D:361:ILE:HG22	1:D:370:PHE:HZ	1.75	0.49
1:D:52:MET:HB3	1:D:78:MET:HE1	1.94	0.49
1:B:317:ILE:HG13	1:B:317:ILE:O	2.12	0.49
1:D:224:LYS:NZ	6:D:387:HOH:O	2.41	0.49
1:B:199:VAL:O	1:B:202:GLU:HA	2.13	0.49
1:D:91:ILE:HD13	1:D:282:MET:HE2	1.89	0.49
1:C:180:ARG:HD2	1:C:206:ILE:HD13	1.94	0.49
1:B:124:TRP:CH2	1:B:181:LEU:HB3	2.47	0.48
1:C:121:HIS:CD2	1:C:370:PHE:HE2	2.31	0.48
1:C:72:GLU:CG	1:C:73:ARG:N	2.76	0.48
1:A:130:ILE:CG2	1:A:159:ILE:CG1	2.91	0.48
1:A:52:MET:HE3	1:A:79:LEU:HD11	1.94	0.48
1:B:97:VAL:HG23	1:B:100:SER:HB3	1.95	0.48
1:D:65:TYR:CE1	1:D:296:ILE:HG22	2.34	0.48
1:B:199:VAL:O	1:B:202:GLU:N	2.46	0.48
1:B:106:GLN:HE22	1:B:342:ARG:HD3	1.74	0.48
1:C:16:GLN:HA	1:C:43:ILE:HD11	1.94	0.48
1:C:181:LEU:HD22	1:C:209:HIS:HB2	1.90	0.48
1:C:3:MET:HE2	1:C:290:ARG:HA	1.95	0.48
1:A:353:MET:HA	1:A:358:ILE:HA	1.95	0.48
1:B:182:VAL:HG12	1:B:183:VAL:N	2.29	0.48
1:C:157:VAL:CG1	1:C:162:THR:OG1	2.62	0.48
1:D:334:ASN:ND2	1:D:345:ASN:HB3	2.29	0.48
1:A:135:ARG:NH1	1:A:135:ARG:CG	2.48	0.48
1:B:240:TYR:CE1	1:B:249:MET:HE3	2.48	0.48
1:D:137:LEU:C	1:D:137:LEU:HD12	2.34	0.48
1:B:365:ASN:OD1	1:B:365:ASN:C	2.52	0.48
1:C:107:LEU:O	1:C:343:ARG:NH1	2.45	0.48
1:C:216:GLY:O	1:C:220:ILE:HG23	2.13	0.48
1:C:6:ASN:ND2	1:C:36:LYS:HB3	2.28	0.48
1:D:229:GLY:O	1:D:354:LYS:HE3	2.14	0.48
1:B:11:GLY:HA2	1:B:68:PHE:O	2.13	0.48
1:A:124:TRP:CE2	1:A:181:LEU:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:TYR:CE2	1:C:371:VAL:CG2	2.97	0.47
1:D:349:HIS:HB2	5:D:900:NAG:H82	1.95	0.47
1:A:47:SER:CB	1:A:72:GLU:OE1	2.62	0.47
1:B:135:ARG:NE	1:B:185:ASP:OD1	2.47	0.47
1:B:226:LYS:HD3	1:B:356:ASP:OD1	2.15	0.47
1:B:354:LYS:O	1:B:357:GLY:CA	2.62	0.47
1:D:194:ILE:HG22	1:D:198:ILE:CD1	2.44	0.47
1:A:301:ASN:OD1	1:A:302:ALA:N	2.47	0.47
1:B:106:GLN:NE2	1:B:342:ARG:CD	2.70	0.47
1:B:52:MET:HB2	1:B:78:MET:HE2	1.96	0.47
1:C:171:PHE:CE1	1:C:180:ARG:HB3	2.49	0.47
1:A:159:ILE:HD12	1:A:167:TYR:CZ	2.47	0.47
1:C:124:TRP:CD2	1:C:181:LEU:HB3	2.49	0.47
1:C:195:LEU:O	1:C:198:ILE:HG22	2.14	0.47
1:A:119:ILE:HG23	1:A:124:TRP:HB2	1.97	0.47
1:D:289:LEU:HD13	1:D:296:ILE:CD1	2.44	0.47
1:D:122:TYR:HB3	3:O:2:NAG:H81	1.96	0.47
1:A:190:ARG:HG2	1:A:194:ILE:CD1	2.36	0.47
1:C:263:VAL:CG1	1:C:264:ASP:N	2.67	0.47
1:C:105:LEU:HD21	1:C:323:LEU:HB3	1.95	0.47
1:D:199:VAL:HG23	1:D:200:LYS:N	2.29	0.47
1:C:124:TRP:CE2	1:C:181:LEU:HB3	2.50	0.47
1:D:105:LEU:CD1	1:D:323:LEU:CB	2.93	0.47
1:D:119:ILE:HG23	1:D:124:TRP:HB2	1.97	0.47
1:D:48:ASP:O	1:D:52:MET:HG2	2.14	0.47
1:A:355:HIS:O	1:A:356:ASP:HB2	2.15	0.47
1:D:199:VAL:HA	1:D:202:GLU:HG2	1.97	0.47
1:A:54:TYR:O	1:A:58:SER:HB2	2.15	0.47
1:B:78:MET:SD	1:B:78:MET:C	2.93	0.47
1:C:12:LEU:HD22	1:C:52:MET:CE	2.45	0.47
1:A:78:MET:C	1:A:78:MET:SD	2.93	0.46
1:C:149:GLU:HG3	1:C:150:LYS:HG3	1.97	0.46
1:C:304:ASP:OD2	6:C:406:HOH:O	2.20	0.46
1:B:26:PHE:CD1	1:B:252:TRP:HB3	2.47	0.46
1:C:280:LYS:HE3	1:C:328:PHE:HE1	1.80	0.46
1:D:354:LYS:O	1:D:357:GLY:N	2.49	0.46
1:A:8:GLN:HE21	1:A:38:LEU:HD23	1.79	0.46
1:B:126:THR:HG22	1:B:153:GLN:HB2	1.97	0.46
1:C:287:GLN:O	1:C:291:ARG:HG2	2.15	0.46
1:C:86:LEU:O	1:C:87:HIS:HB2	2.16	0.46
1:D:158:ASN:HB3	1:D:161:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:GLU:OE1	1:C:20:GLU:N	2.34	0.46
1:A:130:ILE:HG21	1:A:159:ILE:HD11	1.94	0.46
1:A:76:VAL:HG13	1:A:77:ASN:N	2.31	0.46
1:C:171:PHE:C	1:C:173:ASP:N	2.66	0.46
1:C:108:ARG:HA	1:C:109:PRO:HD3	1.81	0.46
1:D:108:ARG:HH12	1:D:187:GLU:CD	2.19	0.46
1:D:231:ASN:HA	1:D:354:LYS:HG3	1.98	0.46
1:C:105:LEU:CD2	1:C:323:LEU:HB3	2.45	0.46
1:D:250:GLN:O	1:D:254:THR:HG23	2.16	0.46
1:D:296:ILE:CG2	1:D:297:SER:N	2.79	0.46
1:D:55:ARG:HD3	1:D:55:ARG:HA	1.75	0.46
1:B:206:ILE:HG13	1:B:206:ILE:H	1.57	0.45
1:B:70:PHE:HE1	1:B:93:PRO:HG2	1.77	0.45
1:C:280:LYS:HE3	1:C:328:PHE:CE1	2.51	0.45
1:C:276:TYR:CE2	1:C:280:LYS:CD	2.98	0.45
1:C:222:LEU:HD22	1:C:353:MET:HE1	1.97	0.45
1:C:71:TYR:CD2	1:C:90:PHE:CE2	2.88	0.45
1:D:129:TYR:CD2	1:D:140:LEU:HD13	2.51	0.45
1:B:72:GLU:CG	1:B:73:ARG:N	2.80	0.45
1:B:222:LEU:O	1:B:223:ASN:OD1	2.34	0.45
1:B:267:ARG:HA	1:B:268:PRO:HD3	1.77	0.45
1:A:130:ILE:CG2	1:A:159:ILE:CD1	2.91	0.45
1:B:354:LYS:HE2	1:B:359:ARG:HH12	1.82	0.45
1:B:71:TYR:CD2	1:B:90:PHE:HE2	2.32	0.45
1:C:352:GLU:OE1	1:C:361:ILE:CD1	2.65	0.45
1:D:361:ILE:HG22	1:D:370:PHE:CZ	2.52	0.45
1:A:219:ASP:OD1	1:A:267:ARG:NH1	2.50	0.44
1:A:52:MET:HB3	1:A:78:MET:CE	2.47	0.44
1:B:239:ASN:ND2	1:B:242:ASP:OD1	2.50	0.44
1:D:26:PHE:CE2	1:D:252:TRP:CB	2.98	0.44
1:D:71:TYR:CD2	1:D:90:PHE:CE2	2.94	0.44
1:B:174:LEU:HD23	1:B:180:ARG:CD	2.37	0.44
1:A:319:ILE:HD12	1:A:319:ILE:N	2.32	0.44
1:A:366:GLU:OE2	6:A:398:HOH:O	2.21	0.44
1:D:135:ARG:NH1	1:D:135:ARG:CG	2.61	0.44
1:D:26:PHE:CZ	1:D:252:TRP:CB	2.68	0.44
1:A:60:PHE:O	1:A:298:ARG:NH2	2.50	0.44
1:B:249:MET:O	1:B:253:ARG:HG3	2.18	0.44
1:C:25:ARG:NH2	1:C:262:ARG:HH12	2.14	0.44
1:A:169:MET:CE	1:C:148:ALA:O	2.65	0.44
1:D:157:VAL:HG13	1:D:162:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:HIS:HD2	1:C:370:PHE:CE2	2.35	0.44
1:D:97:VAL:CG2	1:D:100:SER:HB3	2.47	0.44
1:A:373:ALA:O	1:A:375:LEU:CD1	2.62	0.43
1:C:124:TRP:HZ2	1:C:209:HIS:CB	2.28	0.43
1:A:70:PHE:CE1	1:A:93:PRO:HG2	2.53	0.43
1:A:55:ARG:HA	1:A:55:ARG:HD3	1.81	0.43
1:B:250:GLN:CA	1:B:253:ARG:NH2	2.82	0.43
1:B:352:GLU:OE1	1:B:361:ILE:HD13	2.19	0.43
1:B:78:MET:CE	1:B:79:LEU:HG	2.49	0.43
1:B:71:TYR:HD2	1:B:90:PHE:CE2	2.31	0.43
1:D:369:LYS:HD3	1:D:369:LYS:HA	1.75	0.43
1:C:353:MET:HA	1:C:357:GLY:O	2.17	0.43
1:C:3:MET:HG3	1:C:4:PRO:O	2.18	0.43
1:D:195:LEU:HD11	1:D:220:ILE:HG23	2.00	0.43
1:B:322:ALA:O	1:B:326:VAL:HG23	2.19	0.43
1:C:200:LYS:H	1:C:200:LYS:HG3	1.66	0.43
4:M:3:BMA:H4	4:M:4:MAN:H2	2.00	0.43
1:D:16:GLN:HA	1:D:43:ILE:CD1	2.48	0.43
1:C:276:TYR:CE2	1:C:280:LYS:HD2	2.54	0.43
1:C:352:GLU:OE1	1:C:361:ILE:HG12	2.18	0.43
1:A:76:VAL:HG21	1:A:97:VAL:HG21	2.00	0.43
1:C:20:GLU:OE2	1:C:269:LYS:NZ	2.51	0.43
1:D:339:GLU:H	1:D:339:GLU:CD	2.22	0.43
1:D:71:TYR:HE2	1:D:92:THR:HG21	1.83	0.43
1:D:349:HIS:CB	5:D:900:NAG:H82	2.49	0.43
1:C:226:LYS:HE3	1:C:356:ASP:C	2.39	0.43
1:A:371:VAL:O	1:A:371:VAL:HG23	2.19	0.43
1:C:352:GLU:HB2	1:C:361:ILE:HG13	2.01	0.43
1:B:16:GLN:HA	1:B:43:ILE:HD11	2.01	0.42
1:C:224:LYS:NZ	1:C:225:PHE:CE1	2.83	0.42
1:D:7:ILE:HG12	1:D:35:PRO:HB2	2.01	0.42
1:A:216:GLY:O	1:A:220:ILE:HG12	2.19	0.42
1:A:175:GLU:O	1:A:176:LYS:CB	2.51	0.42
1:A:194:ILE:O	1:A:198:ILE:HG12	2.20	0.42
1:C:355:HIS:HB2	1:C:356:ASP:H	1.68	0.42
1:D:180:ARG:HD2	1:D:180:ARG:N	2.34	0.42
1:D:222:LEU:HD13	1:D:353:MET:HE1	2.02	0.42
1:D:218:MET:C	1:D:267:ARG:HH22	2.23	0.42
1:C:17:GLN:HE22	2:N:1:NAG:C8	2.32	0.42
1:A:135:ARG:NH2	1:A:185:ASP:OD1	2.52	0.42
1:C:247:ARG:O	1:C:250:GLN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ARG:HA	1:C:335:VAL:O	2.20	0.42
1:D:249:MET:O	1:D:253:ARG:HB2	2.19	0.42
1:A:191:LEU:HD23	1:A:220:ILE:CG1	2.47	0.42
1:D:26:PHE:CE2	1:D:252:TRP:CG	3.07	0.42
1:D:363:TYR:CE2	1:D:371:VAL:CG2	3.02	0.42
1:B:128:VAL:HB	1:B:182:VAL:HG13	2.02	0.42
1:B:131:TYR:HD1	1:B:132:ASP:O	2.02	0.42
1:A:137:LEU:HD11	1:C:141:GLN:OE1	2.19	0.42
1:D:137:LEU:HD12	1:D:138:SER:N	2.34	0.42
1:B:2:ALA:O	1:B:295:ASP:HA	2.20	0.42
1:C:96:PRO:CD	1:C:108:ARG:HD2	2.30	0.42
1:A:135:ARG:HG3	1:A:135:ARG:O	2.19	0.41
1:C:25:ARG:CZ	1:C:262:ARG:HH12	2.33	0.41
1:D:18:SER:OG	1:D:21:HIS:HD2	2.03	0.41
1:B:178:LYS:HB3	1:B:179:GLU:H	1.61	0.41
1:C:27:ALA:HB2	1:C:276:TYR:CD1	2.55	0.41
1:C:12:LEU:HD22	1:C:52:MET:HE2	2.02	0.41
1:A:71:TYR:CD2	1:A:90:PHE:HE2	2.27	0.41
1:B:171:PHE:CG	1:B:174:LEU:HD12	2.56	0.41
1:D:65:TYR:CE1	1:D:296:ILE:HG21	2.54	0.41
1:D:122:TYR:OH	1:D:361:ILE:HD13	2.20	0.41
1:C:124:TRP:CE2	1:C:181:LEU:HD13	2.55	0.41
1:D:221:ASP:OD2	1:D:223:ASN:ND2	2.53	0.41
1:D:298:ARG:HD2	1:D:313:TRP:CE2	2.55	0.41
1:A:284:GLU:HB3	1:A:326:VAL:HG22	2.03	0.41
1:B:11:GLY:HA3	1:B:41:ILE:CG2	2.48	0.41
1:B:208:TYR:HB3	1:B:210:TYR:CE2	2.55	0.41
1:C:121:HIS:O	1:C:121:HIS:ND1	2.53	0.41
1:C:308:ASN:HA	1:C:309:PRO:HA	1.81	0.41
1:D:217:PHE:CD1	1:D:234:GLY:HA3	2.55	0.41
1:B:350:VAL:HB	1:B:361:ILE:CG2	2.49	0.41
1:C:132:ASP:HB3	1:C:135:ARG:HG2	2.03	0.41
1:D:319:ILE:N	1:D:319:ILE:HD12	2.36	0.41
1:B:217:PHE:C	1:B:219:ASP:N	2.74	0.41
1:B:350:VAL:HB	1:B:361:ILE:HG23	2.02	0.41
1:D:26:PHE:CE1	1:D:252:TRP:CB	2.90	0.41
1:A:195:LEU:CD2	1:A:225:PHE:CE2	2.94	0.41
1:A:350:VAL:HG23	1:A:363:TYR:HA	2.01	0.41
1:A:47:SER:HB3	1:A:72:GLU:OE1	2.21	0.41
1:B:106:GLN:HE22	1:B:342:ARG:CD	2.32	0.41
1:B:3:MET:CE	1:B:289:LEU:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:TYR:O	1:B:280:LYS:HD3	2.21	0.41
1:A:124:TRP:CZ2	1:A:181:LEU:HB3	2.56	0.40
1:A:317:ILE:O	1:A:321:ARG:HG3	2.21	0.40
1:A:74:ARG:NH1	2:E:2:NAG:C8	2.82	0.40
1:A:171:PHE:HA	1:A:174:LEU:HB3	2.01	0.40
1:C:33:GLU:HB2	1:C:287:GLN:NE2	2.35	0.40
1:B:198:ILE:O	1:B:201:LEU:HB2	2.22	0.40
1:B:240:TYR:CD1	1:B:249:MET:CE	3.05	0.40
1:C:121:HIS:HD2	1:C:370:PHE:HE2	1.68	0.40
1:C:44:VAL:HG22	1:C:45:ASN:N	2.36	0.40
1:D:170:LEU:C	1:D:170:LEU:HD12	2.41	0.40
1:D:352:GLU:OE1	1:D:359:ARG:NH2	2.54	0.40
1:A:173:ASP:OD2	1:A:173:ASP:N	2.54	0.40
1:A:73:ARG:O	1:A:76:VAL:HG12	2.21	0.40
1:C:171:PHE:C	1:C:173:ASP:H	2.24	0.40
1:D:118:ILE:HD11	1:D:350:VAL:HG21	2.03	0.40
1:D:354:LYS:O	1:D:355:HIS:C	2.59	0.40
1:C:127:PHE:HB2	1:C:181:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/384 (95%)	354 (97%)	12 (3%)	0	100	100
1	B	362/384 (94%)	341 (94%)	20 (6%)	1 (0%)	41	61
1	C	370/384 (96%)	350 (95%)	19 (5%)	1 (0%)	41	61
1	D	363/384 (94%)	342 (94%)	21 (6%)	0	100	100
All	All	1461/1536 (95%)	1387 (95%)	72 (5%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	218	MET
1	C	263	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	322/336 (96%)	316 (98%)	6 (2%)	57 80
1	B	320/336 (95%)	318 (99%)	2 (1%)	86 95
1	C	326/336 (97%)	318 (98%)	8 (2%)	47 73
1	D	320/336 (95%)	311 (97%)	9 (3%)	43 70
All	All	1288/1344 (96%)	1263 (98%)	25 (2%)	57 80

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLU
1	A	106	GLN
1	A	135	ARG
1	A	250	GLN
1	A	331	LEU
1	A	356	ASP
1	B	252	TRP
1	B	299	ARG
1	C	98	ASP
1	C	120	ASP
1	C	121	HIS
1	C	132	ASP
1	C	295	ASP
1	C	326	VAL
1	C	329	GLU
1	C	355	HIS
1	D	38	LEU
1	D	135	ARG
1	D	150	LYS
1	D	153	GLN

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Mol	Chain	Res	Type
1	D	164	GLU
1	D	173	ASP
1	D	252	TRP
1	D	253	ARG
1	D	354	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	B	141	GLN
1	B	197	GLN
1	B	204	ASN
1	B	349	HIS
1	B	355	HIS
1	C	6	ASN
1	C	17	GLN
1	C	355	HIS
1	D	17	GLN
1	D	141	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

32 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	E	1	1,2	14,14,15	0.84	0	17,19,21	1.57	3 (17%)
2	NAG	E	2	2	14,14,15	0.51	0	17,19,21	2.24	2 (11%)
2	BMA	E	3	2	11,11,12	0.53	0	15,15,17	1.68	5 (33%)
3	NAG	F	1	1,3	14,14,15	0.62	0	17,19,21	0.73	0
3	NAG	F	2	3	14,14,15	0.61	0	17,19,21	2.21	7 (41%)
3	NAG	G	1	1,3	14,14,15	0.75	0	17,19,21	1.04	0
3	NAG	G	2	3	14,14,15	0.60	0	17,19,21	1.20	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.50	0	17,19,21	1.39	2 (11%)
2	NAG	H	2	2	14,14,15	0.51	0	17,19,21	1.36	2 (11%)
2	BMA	H	3	2	11,11,12	0.57	0	15,15,17	1.33	3 (20%)
3	NAG	I	1	1,3	14,14,15	0.65	0	17,19,21	2.32	5 (29%)
3	NAG	I	2	3	14,14,15	0.57	0	17,19,21	1.07	3 (17%)
3	NAG	J	1	1,3	14,14,15	0.68	0	17,19,21	1.46	2 (11%)
3	NAG	J	2	3	14,14,15	0.41	0	17,19,21	1.88	3 (17%)
3	NAG	K	1	1,3	14,14,15	0.71	0	17,19,21	1.53	3 (17%)
3	NAG	K	2	3	14,14,15	0.56	0	17,19,21	1.24	1 (5%)
3	NAG	L	1	1,3	14,14,15	0.62	0	17,19,21	1.09	2 (11%)
3	NAG	L	2	3	14,14,15	0.56	0	17,19,21	1.37	2 (11%)
4	NAG	M	1	1,4	14,14,15	0.66	0	17,19,21	1.32	2 (11%)
4	NAG	M	2	4	14,14,15	0.69	0	17,19,21	1.04	0
4	BMA	M	3	4	11,11,12	0.50	0	15,15,17	1.08	1 (6%)
4	MAN	M	4	4	11,11,12	0.72	0	15,15,17	2.03	5 (33%)
4	MAN	M	5	4	11,11,12	0.77	0	15,15,17	1.59	4 (26%)
4	MAN	M	6	4	11,11,12	0.60	0	15,15,17	1.04	1 (6%)
4	MAN	M	7	4	11,11,12	0.60	0	15,15,17	1.26	3 (20%)
2	NAG	N	1	1,2	14,14,15	0.67	0	17,19,21	1.99	4 (23%)
2	NAG	N	2	2	14,14,15	0.69	0	17,19,21	1.64	6 (35%)
2	BMA	N	3	2	11,11,12	0.60	0	15,15,17	1.65	2 (13%)
3	NAG	O	1	1,3	14,14,15	1.53	1 (7%)	17,19,21	1.28	1 (5%)
3	NAG	O	2	3	14,14,15	0.78	0	17,19,21	2.01	4 (23%)
3	NAG	P	1	1,3	14,14,15	1.51	1 (7%)	17,19,21	1.25	2 (11%)
3	NAG	P	2	3	14,14,15	0.60	0	17,19,21	1.13	2 (11%)

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	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	BMA	M	3	4	-	2/2/19/22	0/1/1/1
4	MAN	M	4	4	-	0/2/19/22	0/1/1/1
4	MAN	M	5	4	-	0/2/19/22	0/1/1/1
4	MAN	M	6	4	-	0/2/19/22	0/1/1/1
4	MAN	M	7	4	-	2/2/19/22	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	BMA	N	3	2	-	0/2/19/22	0/1/1/1
3	NAG	O	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1	NAG	O5-C1	-5.48	1.35	1.43
3	P	1	NAG	O5-C1	-5.37	1.35	1.43

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	C1-O5-C5	8.21	123.31	112.19
3	J	2	NAG	C1-O5-C5	6.32	120.75	112.19
3	I	1	NAG	C1-O5-C5	5.75	119.98	112.19
4	M	4	MAN	C3-C4-C5	4.80	118.80	110.24
2	N	1	NAG	O4-C4-C5	-4.36	98.47	109.30
3	I	1	NAG	C4-C3-C2	4.35	117.40	111.02
3	O	2	NAG	C4-C3-C2	4.33	117.37	111.02
3	O	2	NAG	C2-N2-C7	4.33	129.07	122.90
3	F	2	NAG	C1-O5-C5	4.32	118.05	112.19
2	E	3	BMA	C1-C2-C3	4.05	114.65	109.67
3	F	2	NAG	C3-C4-C5	-4.05	103.02	110.24
2	N	1	NAG	O5-C1-C2	-4.02	104.94	111.29
3	K	1	NAG	O5-C5-C6	3.98	113.44	107.20
2	E	1	NAG	C4-C3-C2	3.98	116.84	111.02
2	H	1	NAG	O5-C5-C6	3.80	113.16	107.20
2	N	1	NAG	C6-C5-C4	-3.71	104.30	113.00
3	L	2	NAG	C1-O5-C5	3.57	117.03	112.19
3	O	1	NAG	O5-C1-C2	-3.34	106.02	111.29
4	M	4	MAN	C2-C3-C4	3.32	116.63	110.89
2	N	1	NAG	C1-O5-C5	3.31	116.68	112.19
4	M	5	MAN	C2-C3-C4	3.27	116.56	110.89
2	N	2	NAG	O5-C5-C4	-3.24	102.94	110.83
4	M	4	MAN	C1-O5-C5	3.24	116.58	112.19
2	E	1	NAG	C1-C2-N2	-3.23	104.96	110.49
3	J	1	NAG	C1-C2-N2	-3.20	105.02	110.49
2	N	3	BMA	O5-C5-C4	-3.20	103.05	110.83
2	H	3	BMA	C2-C3-C4	3.19	116.42	110.89
3	K	1	NAG	C3-C4-C5	-3.17	104.58	110.24
3	O	2	NAG	O7-C7-N2	3.04	127.54	121.95
3	G	2	NAG	O5-C5-C6	2.99	111.89	107.20
3	F	2	NAG	O5-C5-C6	2.98	111.88	107.20
3	I	1	NAG	O7-C7-C8	-2.97	116.54	122.06
4	M	5	MAN	C3-C4-C5	2.96	115.52	110.24
2	H	2	NAG	C8-C7-N2	2.94	121.08	116.10
4	M	5	MAN	C1-C2-C3	2.93	113.27	109.67
3	F	2	NAG	O3-C3-C2	2.92	115.51	109.47
3	F	2	NAG	O4-C4-C5	2.92	116.55	109.30
2	E	2	NAG	C4-C3-C2	-2.91	106.75	111.02
3	F	2	NAG	C4-C3-C2	-2.88	106.80	111.02
2	N	3	BMA	O2-C2-C1	-2.85	103.31	109.15
3	I	1	NAG	C2-N2-C7	2.79	126.88	122.90
3	J	2	NAG	C4-C3-C2	-2.71	107.05	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	2	NAG	O5-C5-C6	2.71	111.45	107.20
2	E	3	BMA	O5-C5-C6	2.64	111.35	107.20
3	G	2	NAG	C4-C3-C2	2.53	114.73	111.02
4	M	7	MAN	C3-C4-C5	2.48	114.67	110.24
4	M	4	MAN	C1-C2-C3	2.45	112.68	109.67
4	M	7	MAN	O5-C1-C2	-2.41	107.06	110.77
3	I	2	NAG	O7-C7-C8	-2.37	117.66	122.06
2	H	3	BMA	C3-C4-C5	2.36	114.45	110.24
2	E	3	BMA	O5-C1-C2	2.34	114.38	110.77
4	M	1	NAG	C4-C3-C2	2.29	114.38	111.02
2	H	1	NAG	C4-C3-C2	2.29	114.38	111.02
3	F	2	NAG	C1-C2-N2	2.29	114.40	110.49
3	P	1	NAG	C1-O5-C5	-2.27	109.12	112.19
3	J	1	NAG	O5-C5-C6	2.24	110.71	107.20
3	J	2	NAG	C1-C2-N2	2.21	114.26	110.49
4	M	5	MAN	C1-O5-C5	2.17	115.13	112.19
4	M	1	NAG	O4-C4-C3	-2.17	105.34	110.35
2	N	2	NAG	O4-C4-C3	-2.16	105.34	110.35
4	M	3	BMA	C1-O5-C5	2.15	115.11	112.19
3	L	1	NAG	C1-C2-N2	-2.13	106.85	110.49
3	I	2	NAG	O5-C5-C6	2.12	110.53	107.20
3	P	1	NAG	O5-C1-C2	-2.12	107.94	111.29
2	N	2	NAG	O4-C4-C5	-2.11	104.05	109.30
2	E	1	NAG	O5-C5-C6	2.11	110.51	107.20
3	O	2	NAG	C8-C7-N2	-2.11	112.53	116.10
3	I	2	NAG	C8-C7-N2	2.10	119.66	116.10
4	M	7	MAN	O5-C5-C6	2.10	110.50	107.20
4	M	6	MAN	C1-O5-C5	2.10	115.04	112.19
2	E	3	BMA	C1-O5-C5	2.10	115.03	112.19
2	N	2	NAG	O3-C3-C2	2.09	113.79	109.47
2	E	3	BMA	O5-C5-C4	-2.08	105.76	110.83
2	N	2	NAG	O3-C3-C4	-2.08	105.55	110.35
3	K	1	NAG	C1-C2-N2	-2.07	106.96	110.49
3	P	2	NAG	C2-N2-C7	2.06	125.84	122.90
3	L	2	NAG	C2-N2-C7	2.05	125.82	122.90
3	L	1	NAG	C3-C4-C5	-2.05	106.58	110.24
2	N	2	NAG	C8-C7-N2	2.03	119.54	116.10
3	I	1	NAG	O3-C3-C4	2.03	115.04	110.35
3	K	2	NAG	O7-C7-C8	-2.03	118.30	122.06
2	H	2	NAG	O5-C5-C4	-2.02	105.91	110.83
4	M	4	MAN	O5-C5-C4	2.02	115.74	110.83
2	H	3	BMA	O5-C5-C6	2.01	110.35	107.20

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	1	NAG	C4-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
4	M	7	MAN	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
4	M	7	MAN	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
3	K	1	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
4	M	3	BMA	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
4	M	3	BMA	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6

There are no ring outliers.

12 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1	NAG	3	0
3	I	1	NAG	1	0
2	N	1	NAG	2	0
2	E	2	NAG	2	0
3	K	1	NAG	2	0
4	M	3	BMA	1	0
3	K	2	NAG	1	0

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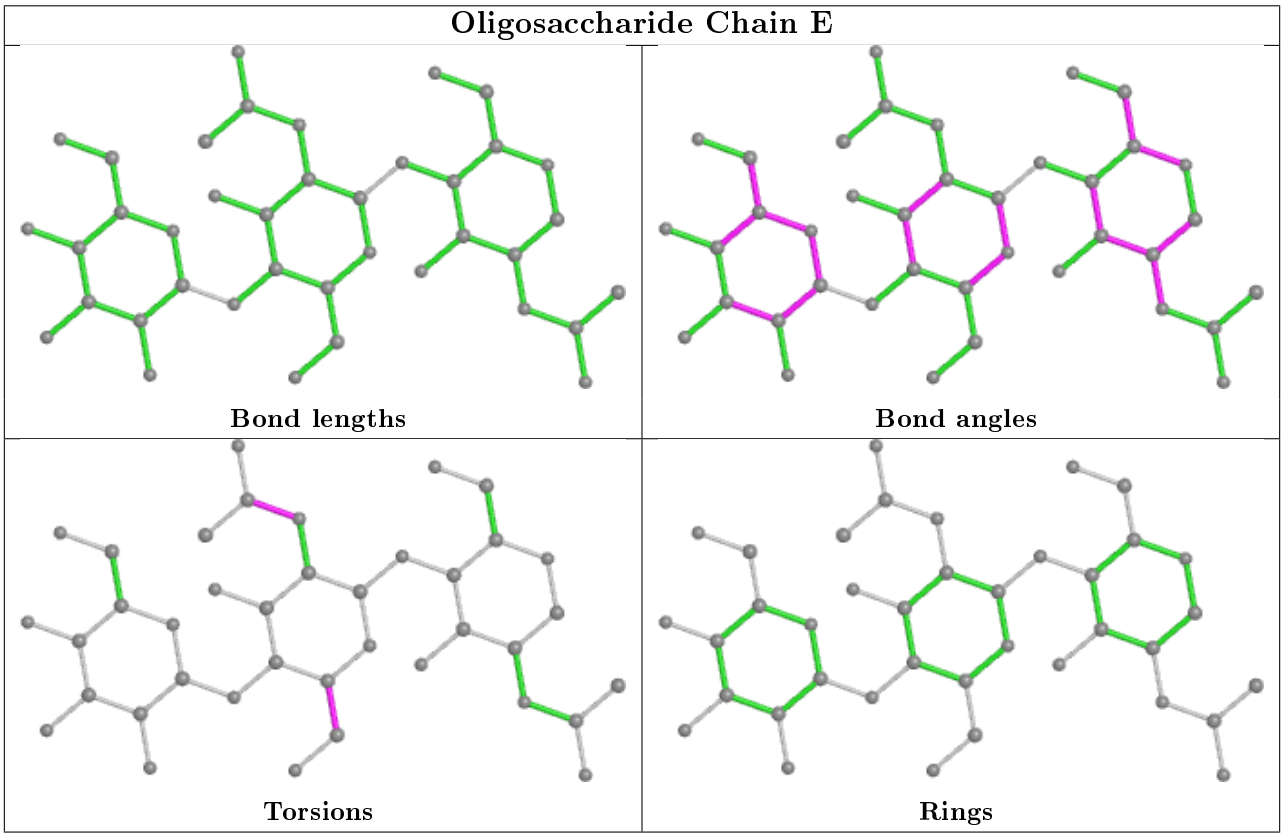
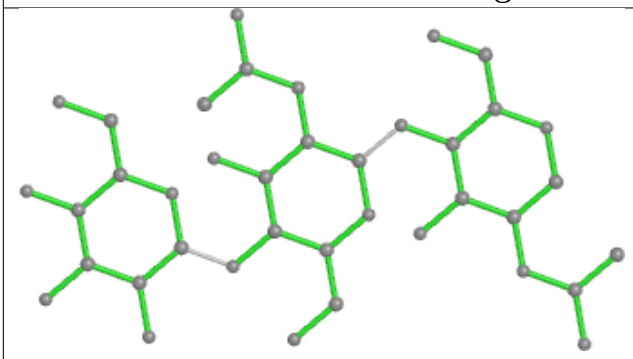
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	4	MAN	1	0
3	F	2	NAG	1	0
2	H	2	NAG	2	0
3	O	2	NAG	1	0
3	F	1	NAG	1	0

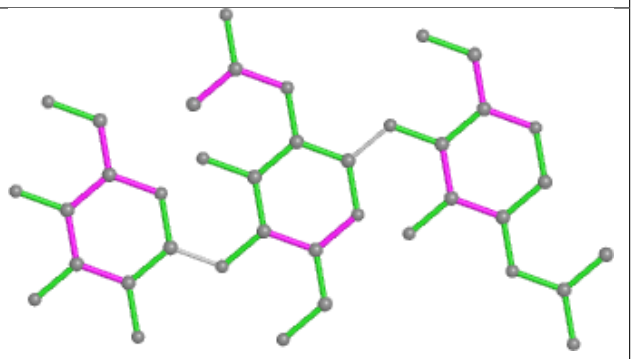
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



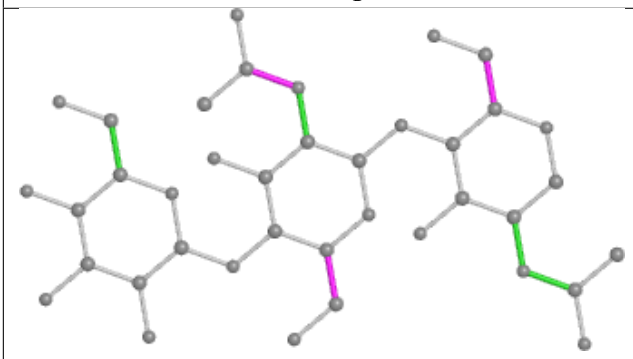
Oligosaccharide Chain H



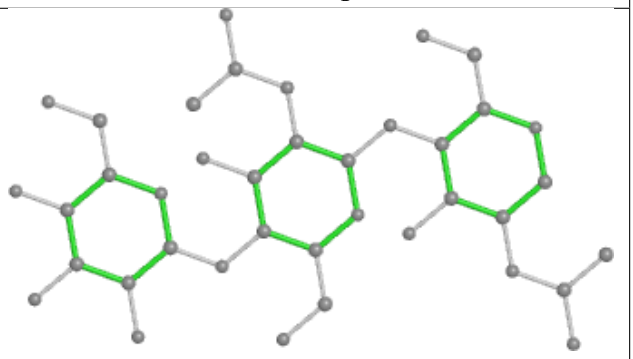
Bond lengths



Bond angles

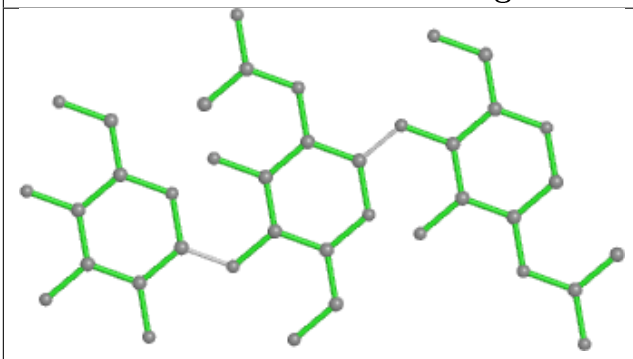


Torsions

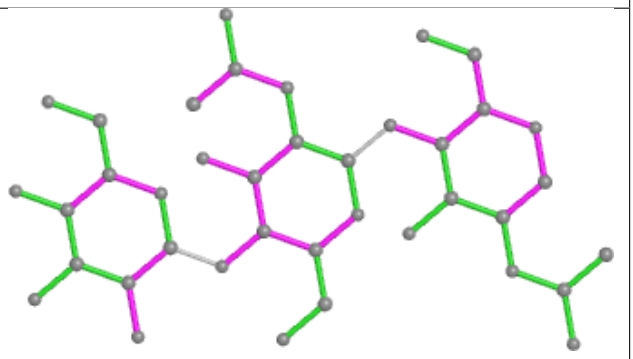


Rings

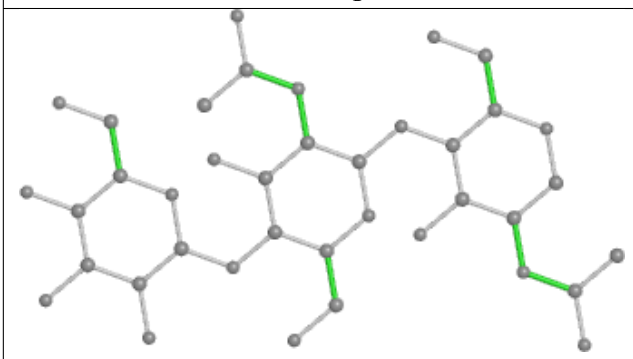
Oligosaccharide Chain N



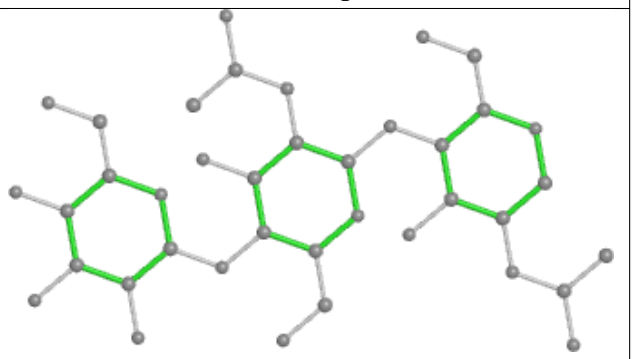
Bond lengths



Bond angles

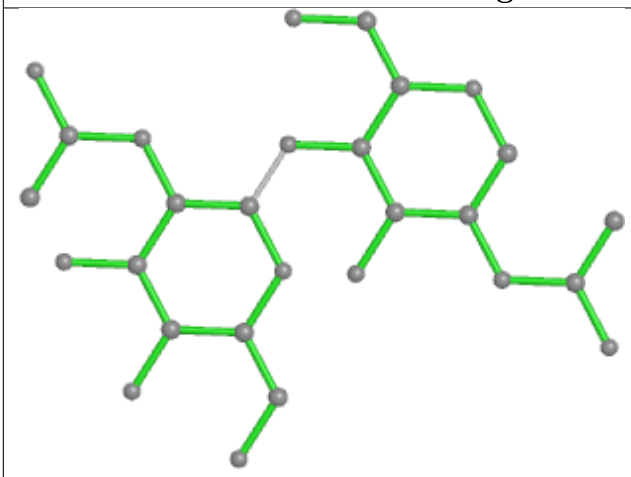


Torsions

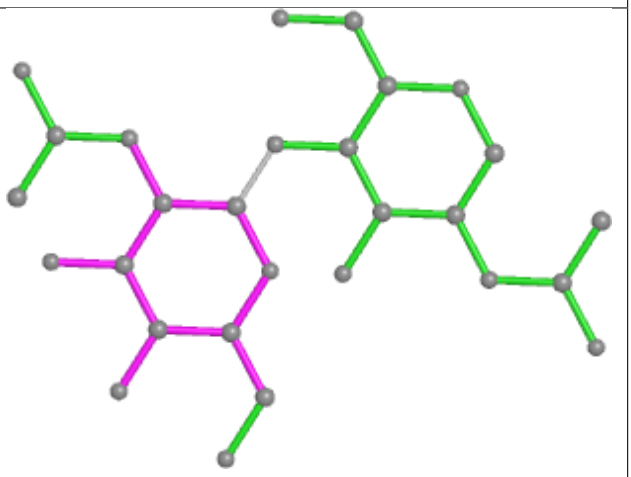


Rings

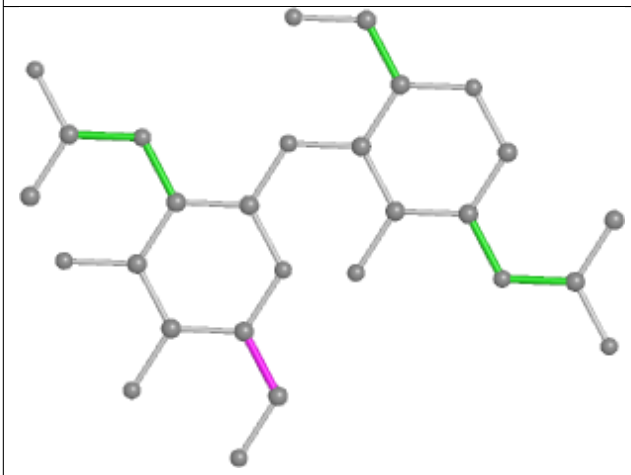
Oligosaccharide Chain F



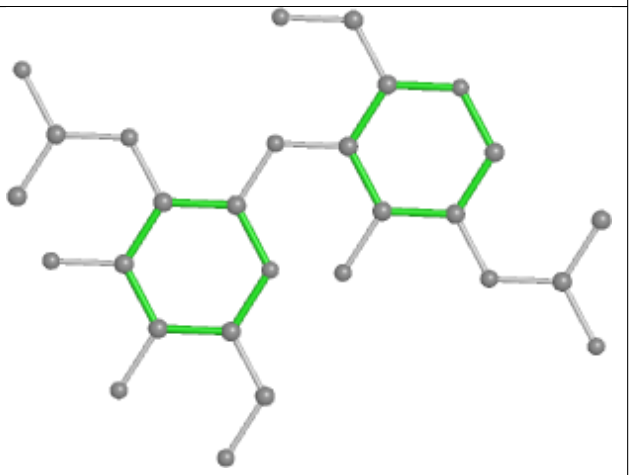
Bond lengths



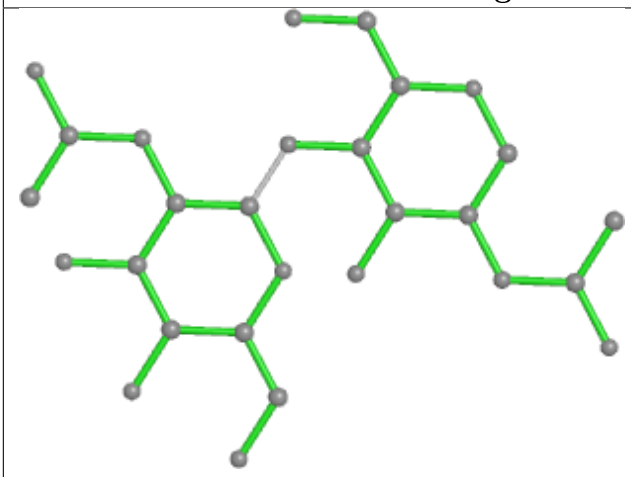
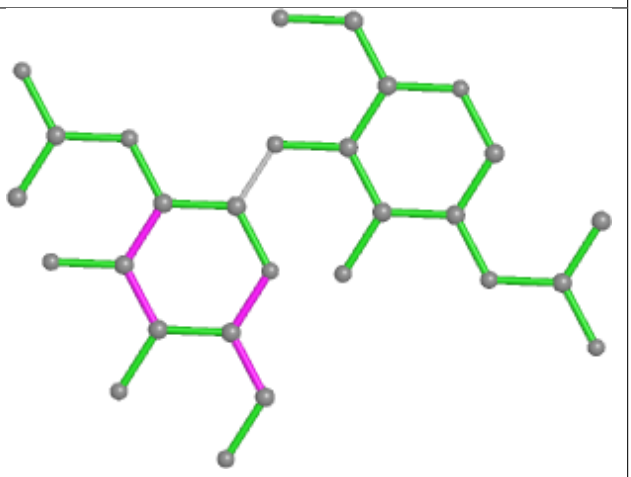
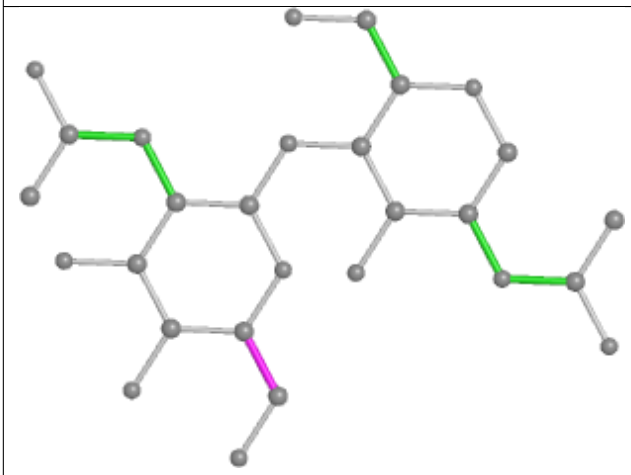
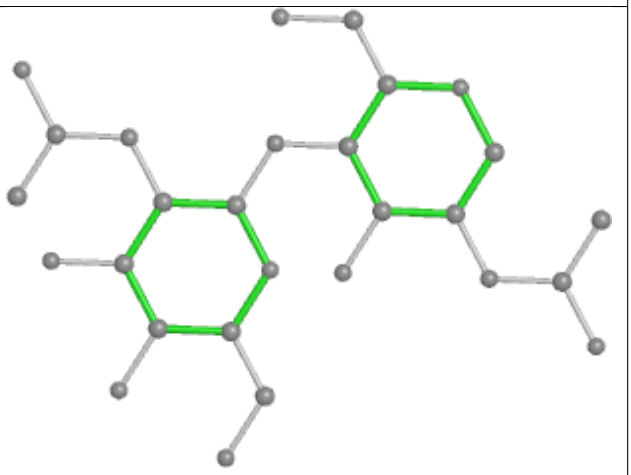
Bond angles



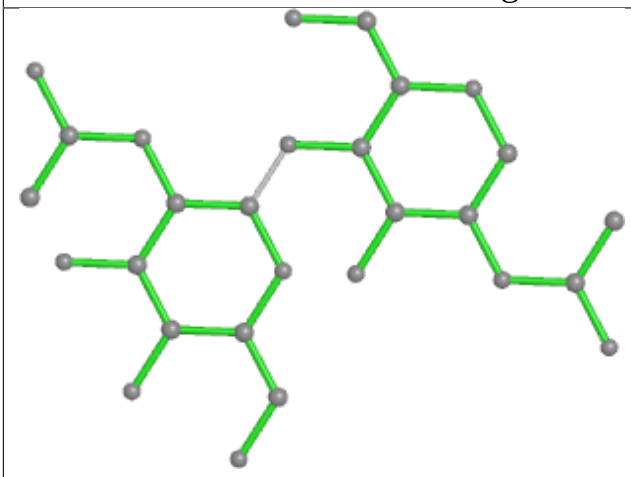
Torsions



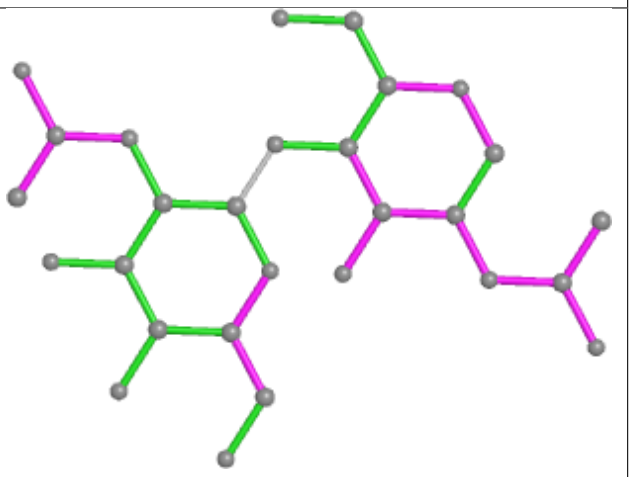
Rings

Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

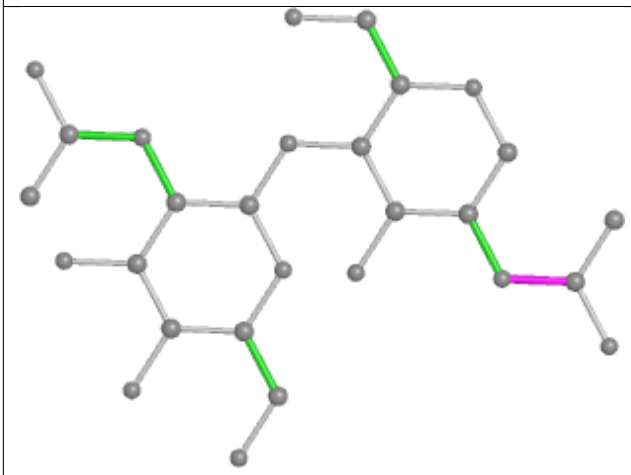
Oligosaccharide Chain I



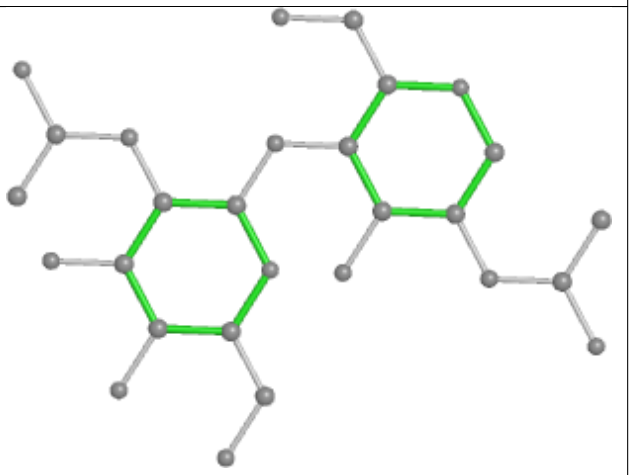
Bond lengths



Bond angles

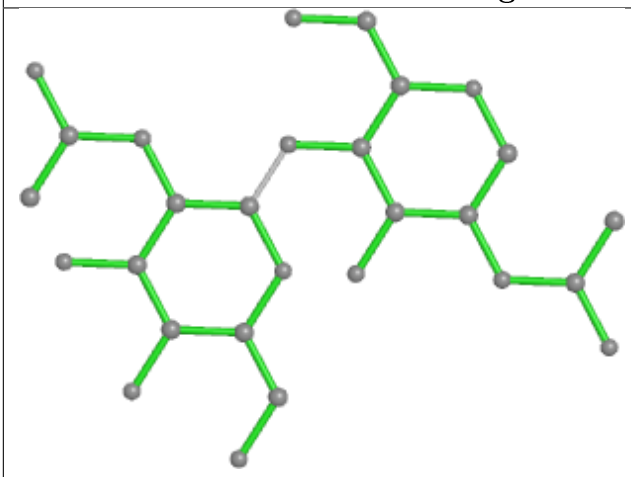


Torsions

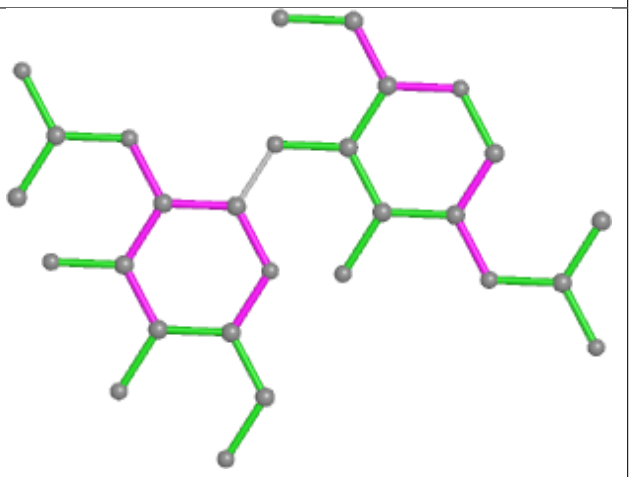


Rings

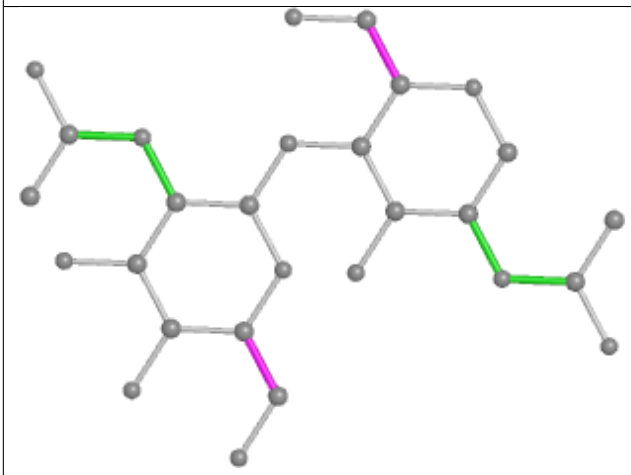
Oligosaccharide Chain J



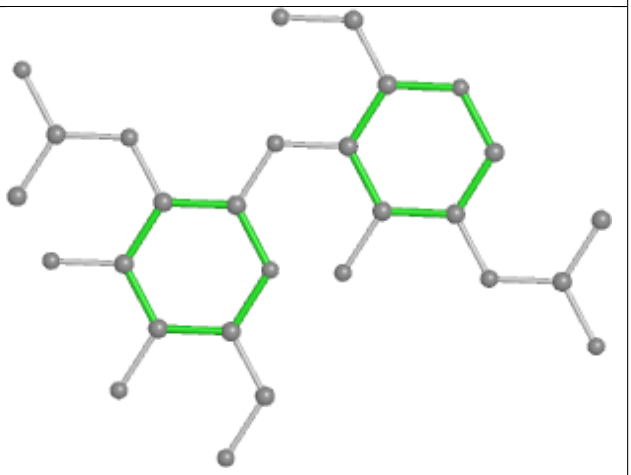
Bond lengths



Bond angles

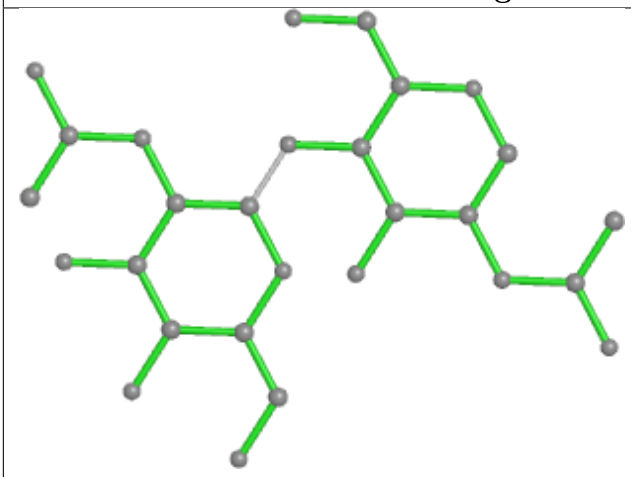


Torsions

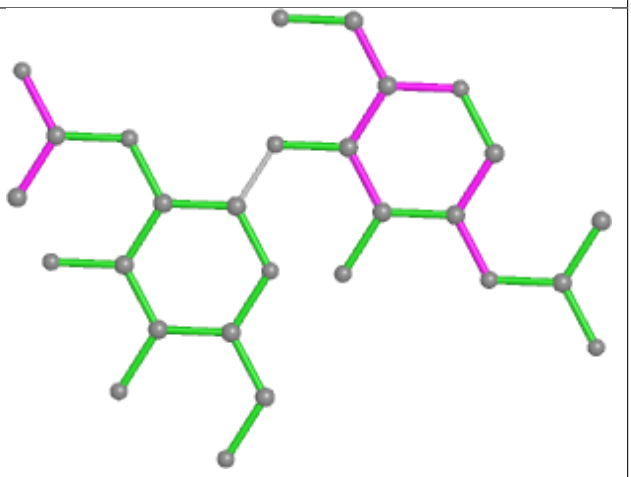


Rings

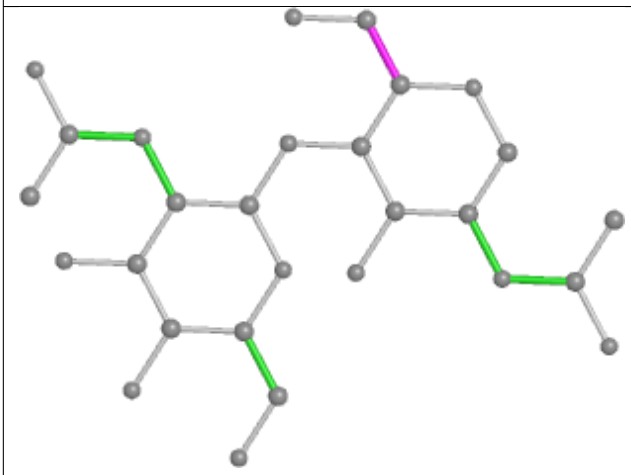
Oligosaccharide Chain K



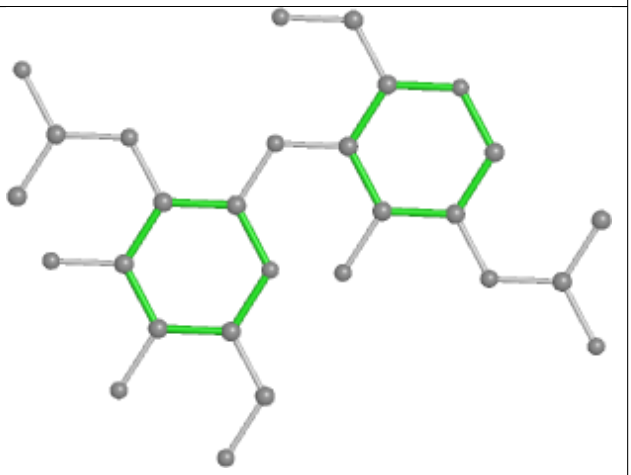
Bond lengths



Bond angles

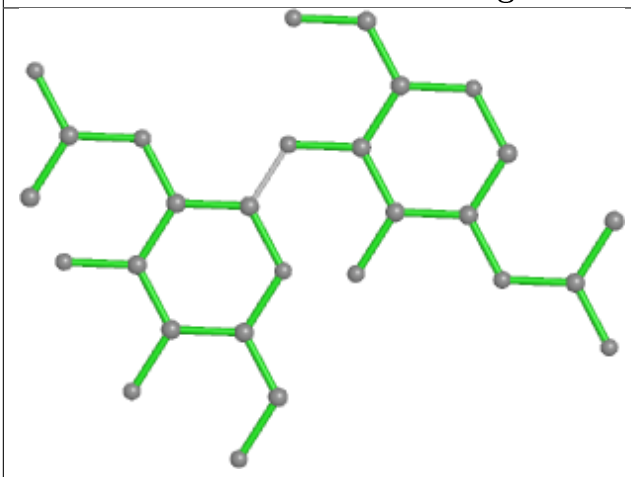


Torsions

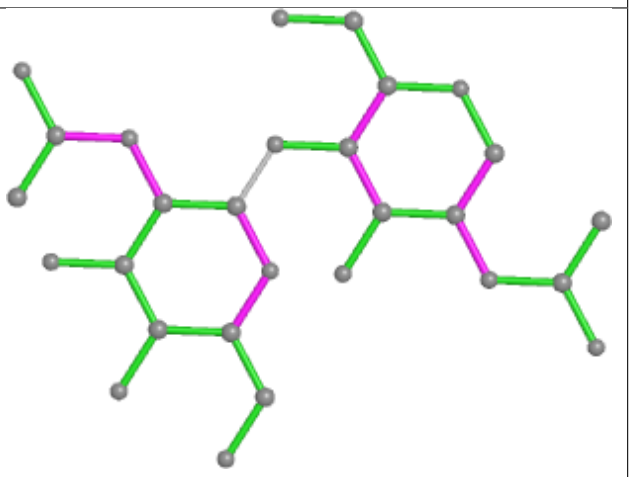


Rings

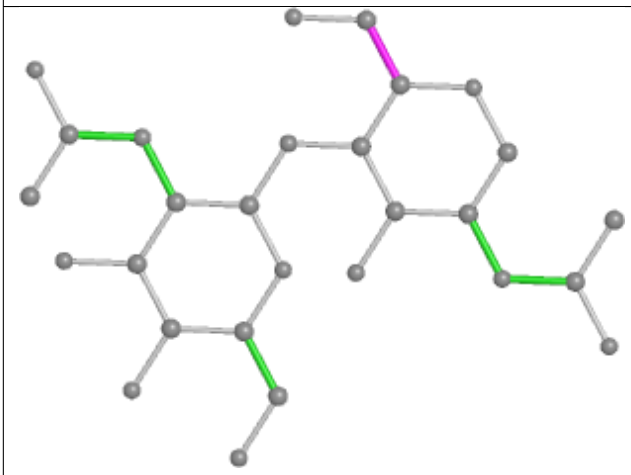
Oligosaccharide Chain L



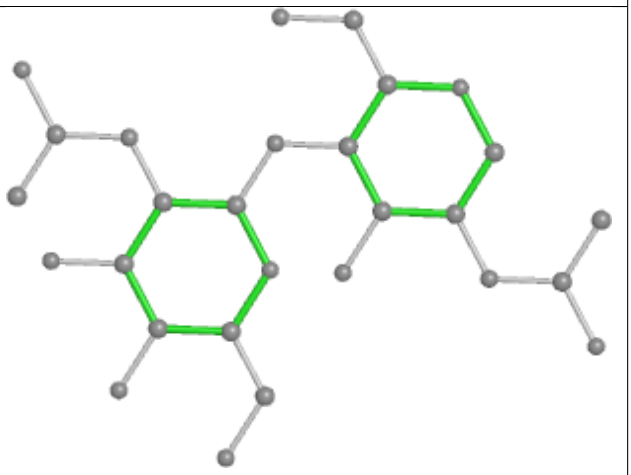
Bond lengths



Bond angles

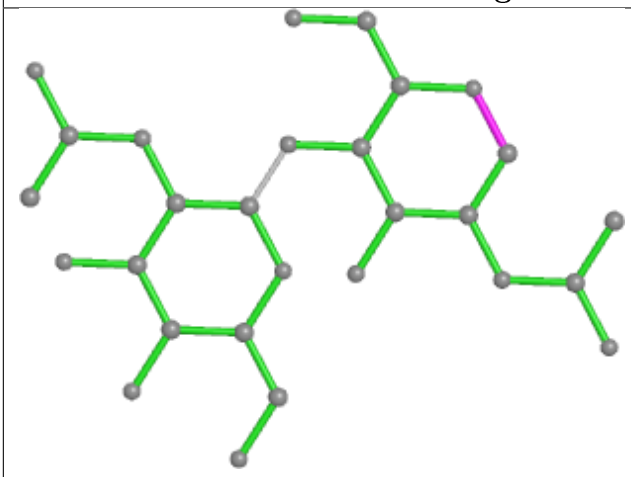


Torsions

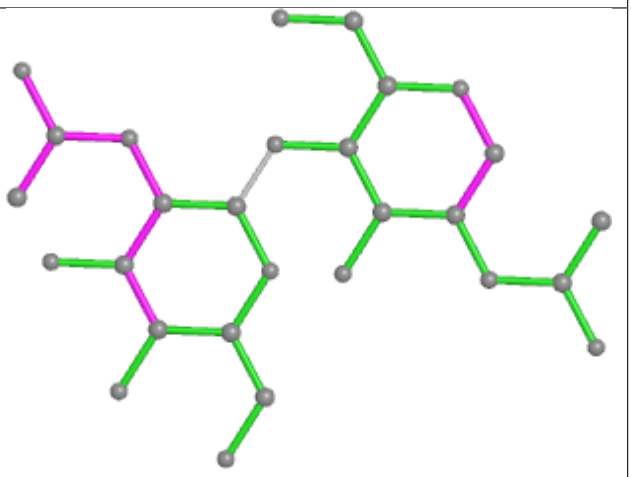


Rings

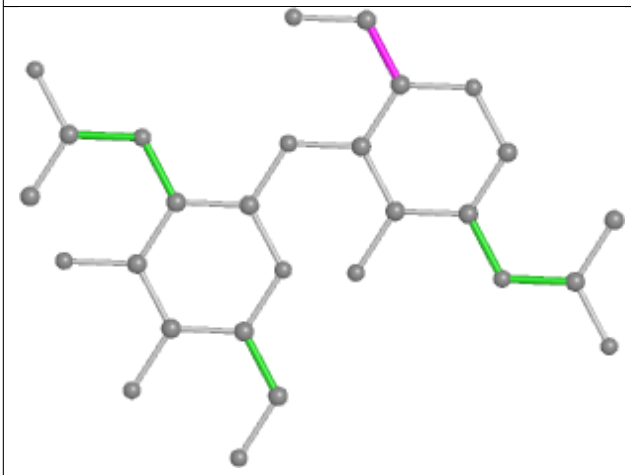
Oligosaccharide Chain O



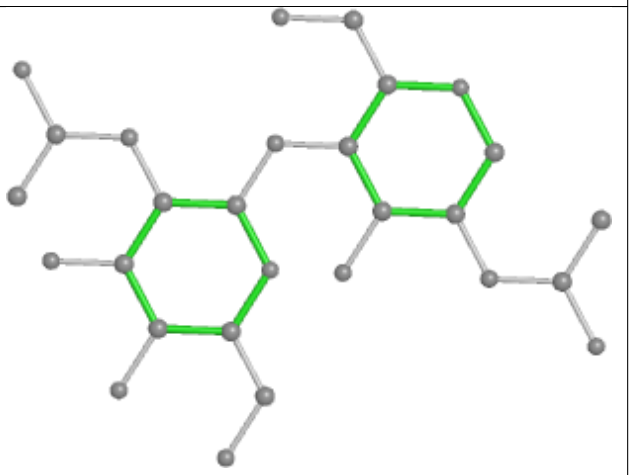
Bond lengths



Bond angles

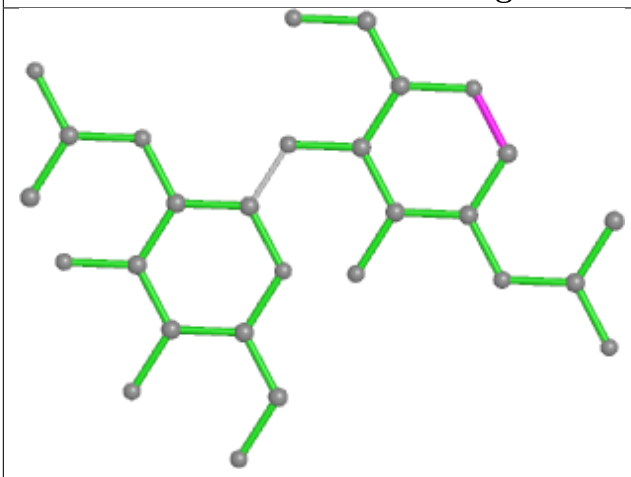


Torsions

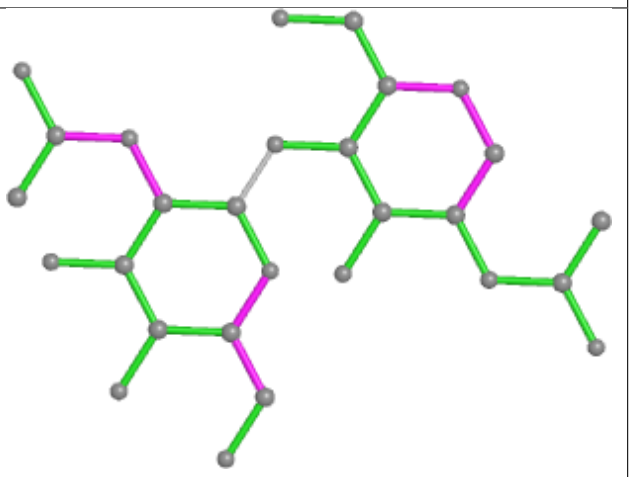


Rings

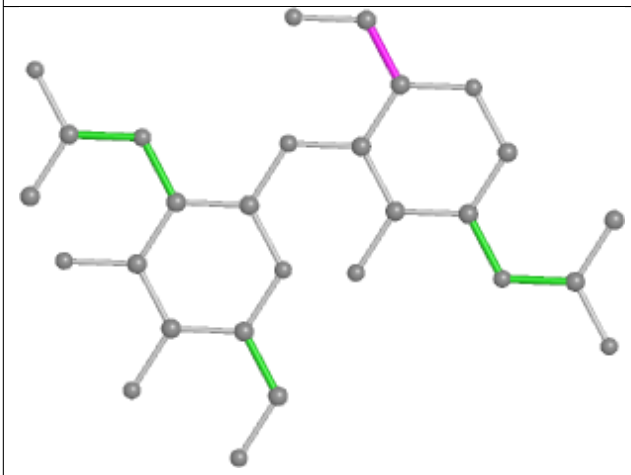
Oligosaccharide Chain P



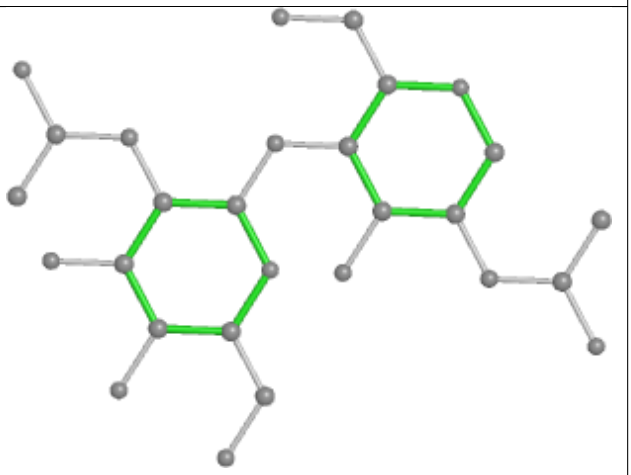
Bond lengths



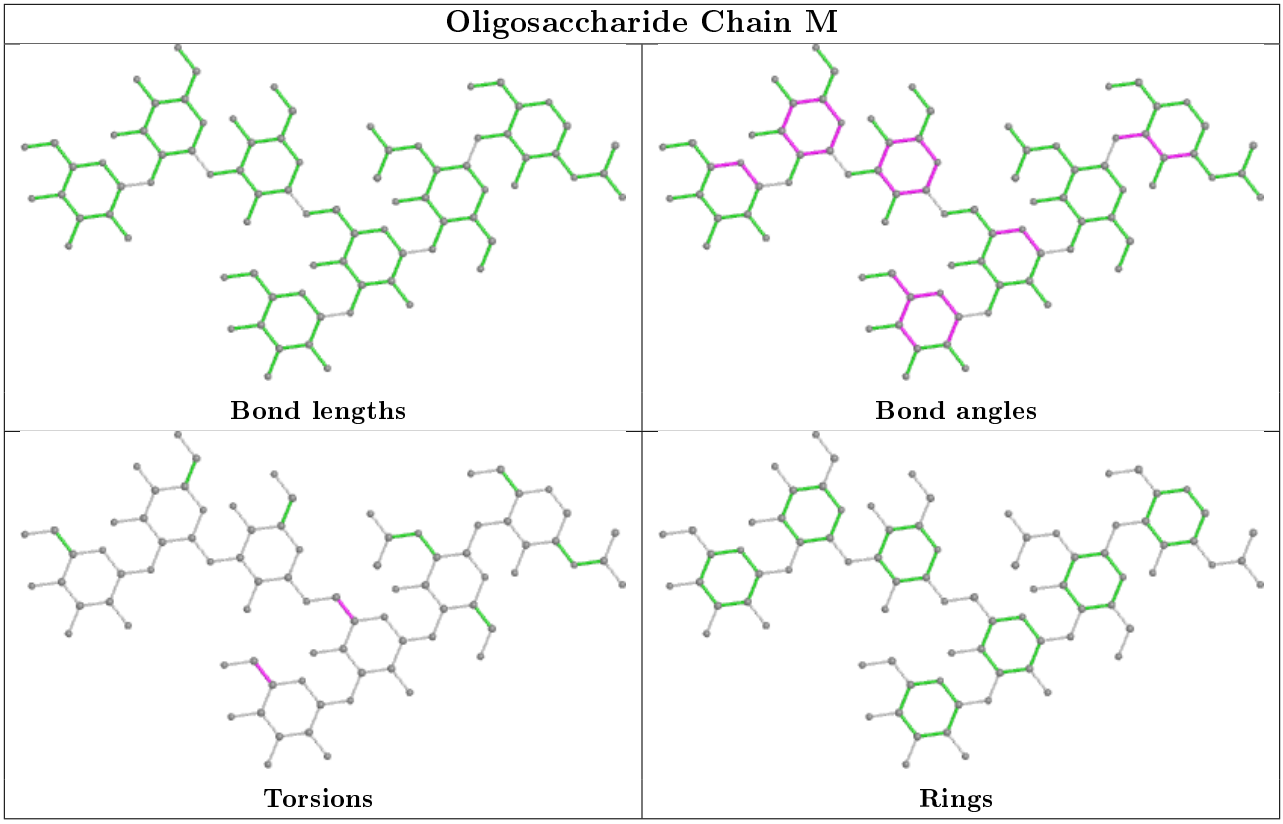
Bond angles



Torsions



Rings



5.6 Ligand geometry

3 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	B	900	1	14,14,15	0.47	0	17,19,21	1.27	2 (11%)
5	NAG	D	900	1	14,14,15	1.27	1 (7%)	17,19,21	3.54	11 (64%)
5	NAG	A	900	1	14,14,15	0.72	0	17,19,21	2.07	6 (35%)

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	B	900	1	-	2/6/23/26	0/1/1/1
5	NAG	D	900	1	-	2/6/23/26	0/1/1/1
5	NAG	A	900	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	900	NAG	O5-C5	4.51	1.52	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	900	NAG	C2-N2-C7	7.40	133.43	122.90
5	D	900	NAG	O5-C1-C2	-6.25	101.42	111.29
5	D	900	NAG	O5-C5-C6	-6.02	97.76	107.20
5	D	900	NAG	O5-C5-C4	-4.56	99.74	110.83
5	D	900	NAG	C1-C2-N2	-4.53	102.75	110.49
5	A	900	NAG	C1-O5-C5	-4.14	106.58	112.19
5	A	900	NAG	C1-C2-N2	-3.78	104.03	110.49
5	A	900	NAG	O5-C1-C2	-3.62	105.57	111.29
5	D	900	NAG	O4-C4-C5	-3.14	101.49	109.30
5	D	900	NAG	O4-C4-C3	-2.41	104.77	110.35
5	D	900	NAG	O7-C7-N2	2.38	126.33	121.95
5	A	900	NAG	C3-C4-C5	2.36	114.45	110.24
5	A	900	NAG	O5-C5-C6	2.28	110.77	107.20
5	B	900	NAG	C4-C3-C2	-2.22	107.76	111.02
5	D	900	NAG	C4-C3-C2	-2.21	107.77	111.02
5	D	900	NAG	C1-O5-C5	2.18	115.14	112.19
5	A	900	NAG	C4-C3-C2	2.16	114.19	111.02
5	B	900	NAG	O4-C4-C5	2.15	114.65	109.30
5	D	900	NAG	C6-C5-C4	-2.13	108.02	113.00

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	900	NAG	C3-C2-N2-C7
5	B	900	NAG	O5-C5-C6-O6
5	A	900	NAG	O5-C5-C6-O6
5	A	900	NAG	C4-C5-C6-O6
5	B	900	NAG	C4-C5-C6-O6
5	D	900	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	900	NAG	1	0
5	D	900	NAG	4	0
5	A	900	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	369/384 (96%)	0.56	36 (9%) 7 7	28, 54, 130, 203	0
1	B	366/384 (95%)	0.71	45 (12%) 4 3	29, 68, 114, 159	0
1	C	372/384 (96%)	0.91	56 (15%) 2 1	29, 63, 133, 199	0
1	D	367/384 (95%)	0.60	40 (10%) 5 5	30, 67, 103, 124	0
All	All	1474/1536 (95%)	0.69	177 (12%) 4 4	28, 62, 119, 203	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	263	VAL	18.4
1	A	172	GLN	10.8
1	C	265	TRP	10.3
1	C	176	LYS	9.2
1	C	178	LYS	8.5
1	C	177	LYS	8.1
1	A	163	THR	7.9
1	C	172	GLN	7.6
1	C	264	ASP	7.5
1	B	357	GLY	7.4
1	B	220	ILE	7.3
1	B	354	LYS	7.2
1	A	375	LEU	7.1
1	C	173	ASP	7.0
1	C	261	THR	6.8
1	B	353	MET	6.8
1	B	223	ASN	6.5
1	A	167	TYR	6.2
1	C	203	LYS	5.7
1	B	180	ARG	5.6
1	C	174	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	258	ARG	5.5
1	C	302	ALA	5.4
1	D	363	TYR	5.2
1	A	180	ARG	5.1
1	B	256	ASP	5.0
1	A	99	THR	5.0
1	C	168	ARG	4.9
1	C	164	GLU	4.9
1	C	204	ASN	4.9
1	A	258	ARG	4.9
1	B	253	ARG	4.9
1	A	171	PHE	4.8
1	B	174	LEU	4.7
1	D	259	ASP	4.7
1	B	221	ASP	4.6
1	C	206	ILE	4.6
1	C	169	MET	4.6
1	B	355	HIS	4.6
1	C	262	ARG	4.5
1	C	205	GLY	4.4
1	C	180	ARG	4.4
1	B	218	MET	4.4
1	C	359	ARG	4.3
1	A	170	LEU	4.3
1	D	267	ARG	4.3
1	B	175	GLU	4.2
1	A	159	ILE	4.2
1	D	257	SER	4.2
1	B	360	LYS	4.2
1	C	258	ARG	4.2
1	C	355	HIS	4.1
1	C	170	LEU	4.1
1	A	98	ASP	4.1
1	D	301	ASN	4.1
1	A	178	LYS	4.1
1	A	259	ASP	4.0
1	B	201	LEU	4.0
1	D	204	ASN	4.0
1	B	179	GLU	4.0
1	B	222	LEU	3.9
1	C	373	ALA	3.9
1	B	226	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	358	ILE	3.8
1	A	169	MET	3.8
1	B	176	LYS	3.8
1	A	173	ASP	3.8
1	C	356	ASP	3.8
1	A	301	ASN	3.8
1	C	175	GLU	3.7
1	A	257	SER	3.7
1	C	167	TYR	3.7
1	A	177	LYS	3.6
1	D	252	TRP	3.6
1	B	266	LYS	3.6
1	C	259	ASP	3.5
1	B	359	ARG	3.5
1	A	374	ALA	3.5
1	C	256	ASP	3.5
1	C	260	HIS	3.4
1	A	189	GLU	3.4
1	B	356	ASP	3.4
1	D	135	ARG	3.3
1	D	175	GLU	3.2
1	C	99	THR	3.2
1	B	178	LYS	3.2
1	B	171	PHE	3.2
1	D	367	ASP	3.2
1	D	137	LEU	3.2
1	A	300	GLY	3.2
1	D	221	ASP	3.2
1	A	217	PHE	3.2
1	C	2	ALA	3.1
1	B	358	ILE	3.1
1	A	358	ILE	3.1
1	D	266	LYS	3.1
1	C	97	VAL	3.1
1	D	226	LYS	3.0
1	B	139	VAL	3.0
1	A	1	GLY	3.0
1	B	229	GLY	3.0
1	D	241	THR	3.0
1	A	161	THR	3.0
1	D	134	ASP	3.0
1	D	140	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	164	GLU	2.9
1	A	266	LYS	2.9
1	D	362	GLY	2.9
1	B	228	SER	2.8
1	D	163	THR	2.8
1	D	227	GLU	2.8
1	D	357	GLY	2.8
1	C	98	ASP	2.8
1	C	252	TRP	2.8
1	A	220	ILE	2.8
1	C	163	THR	2.8
1	B	252	TRP	2.7
1	D	149	GLU	2.7
1	A	166	GLY	2.7
1	B	137	LEU	2.7
1	C	17	GLN	2.7
1	D	302	ALA	2.7
1	D	224	LYS	2.7
1	A	162	THR	2.6
1	D	373	ALA	2.6
1	D	201	LEU	2.6
1	B	134	ASP	2.6
1	D	369	LYS	2.6
1	A	302	ALA	2.6
1	D	250	GLN	2.6
1	C	357	GLY	2.6
1	B	199	VAL	2.6
1	B	195	LEU	2.6
1	C	201	LEU	2.5
1	C	361	ILE	2.5
1	A	256	ASP	2.5
1	D	256	ASP	2.5
1	C	353	MET	2.5
1	A	254	THR	2.5
1	C	254	THR	2.5
1	D	123	LYS	2.5
1	A	158	ASN	2.5
1	B	254	THR	2.5
1	D	178	LYS	2.4
1	D	200	LYS	2.4
1	D	179	GLU	2.4
1	C	240	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	203	LYS	2.4
1	C	293	ARG	2.4
1	D	296	ILE	2.4
1	A	16	GLN	2.4
1	B	352	GLU	2.4
1	B	192	ASN	2.3
1	C	354	LYS	2.3
1	C	225	PHE	2.3
1	B	210	TYR	2.3
1	D	139	VAL	2.3
1	B	3	MET	2.3
1	B	224	LYS	2.2
1	D	190	ARG	2.2
1	B	136	GLY	2.2
1	C	207	GLY	2.2
1	C	247	ARG	2.2
1	C	165	GLU	2.1
1	B	170	LEU	2.1
1	C	280	LYS	2.1
1	C	257	SER	2.1
1	A	215	LEU	2.1
1	B	267	ARG	2.1
1	C	267	ARG	2.1
1	C	358	ILE	2.1
1	C	253	ARG	2.1
1	A	267	ARG	2.0
1	B	258	ARG	2.0
1	C	171	PHE	2.0
1	B	257	SER	2.0
1	B	219	ASP	2.0

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

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

6.3 Carbohydrates (i)

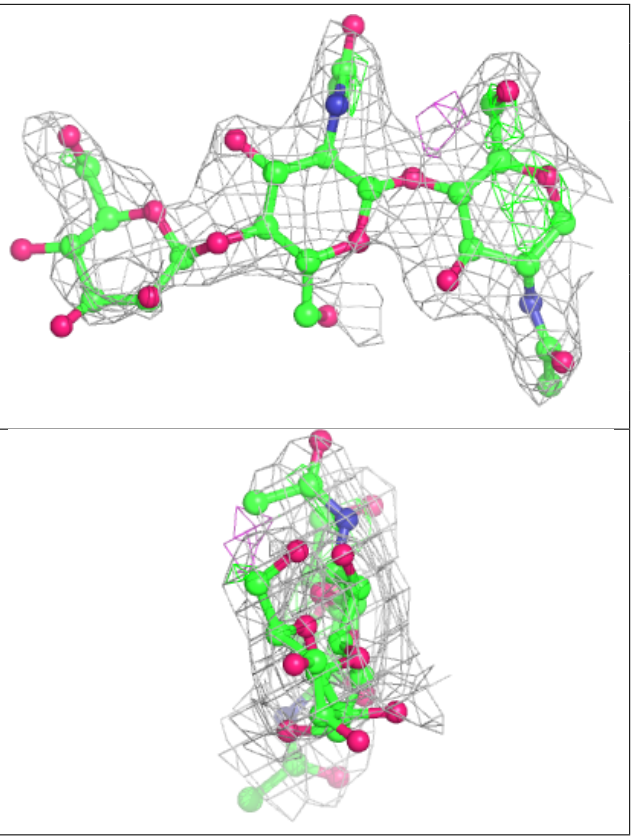
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

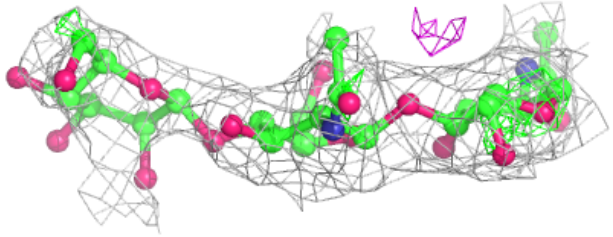
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	M	4	11/12	0.34	0.31	206,210,211,216	0
4	MAN	M	6	11/12	0.48	0.62	224,224,225,225	0
3	NAG	O	2	14/15	0.50	0.42	160,173,175,176	0
2	BMA	E	3	11/12	0.55	0.33	180,183,184,184	0
4	MAN	M	5	11/12	0.57	0.65	220,222,223,223	0
3	NAG	L	1	14/15	0.60	0.30	144,150,157,159	0
2	BMA	H	3	11/12	0.60	0.32	184,186,187,188	0
3	NAG	I	2	14/15	0.62	0.48	102,175,193,194	0
2	NAG	E	2	14/15	0.64	0.29	161,166,171,177	0
3	NAG	F	2	14/15	0.64	0.30	155,158,160,160	0
3	NAG	I	1	14/15	0.71	0.39	129,143,158,168	0
3	NAG	P	2	14/15	0.73	0.26	175,180,184,184	0
4	NAG	M	2	14/15	0.74	0.24	148,152,156,166	0
3	NAG	F	1	14/15	0.74	0.23	129,137,145,150	0
4	MAN	M	7	11/12	0.76	0.21	185,186,187,187	0
3	NAG	J	2	14/15	0.77	0.17	168,172,174,174	0
4	BMA	M	3	11/12	0.77	0.21	175,181,192,200	0
3	NAG	O	1	14/15	0.78	0.32	150,160,163,167	0
3	NAG	L	2	14/15	0.79	0.35	162,164,165,166	0
2	NAG	H	2	14/15	0.79	0.23	163,167,174,179	0
3	NAG	G	2	14/15	0.81	0.22	162,166,168,169	0
3	NAG	K	1	14/15	0.82	0.33	122,135,144,146	0
2	NAG	H	1	14/15	0.83	0.27	130,140,144,154	0
2	NAG	E	1	14/15	0.83	0.23	125,139,144,151	0
2	NAG	N	2	14/15	0.84	0.24	123,126,132,132	0
3	NAG	K	2	14/15	0.84	0.25	152,156,160,161	0
3	NAG	J	1	14/15	0.84	0.20	139,150,154,161	0
2	BMA	N	3	11/12	0.85	0.17	136,138,140,142	0
3	NAG	P	1	14/15	0.86	0.16	146,155,160,168	0
4	NAG	M	1	14/15	0.86	0.27	127,133,139,143	0
2	NAG	N	1	14/15	0.87	0.29	109,119,125,127	0
3	NAG	G	1	14/15	0.89	0.23	129,137,145,153	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 E:

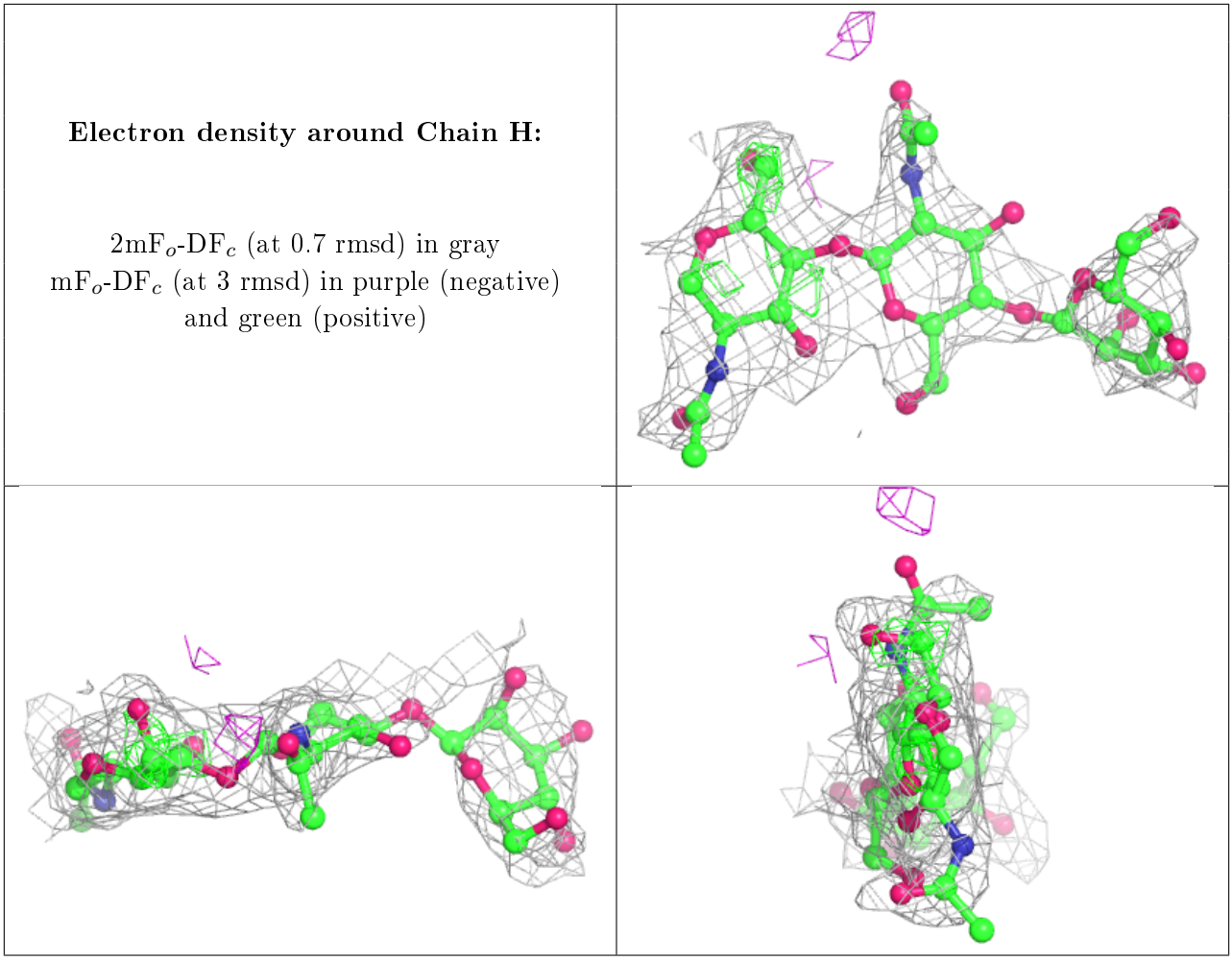
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





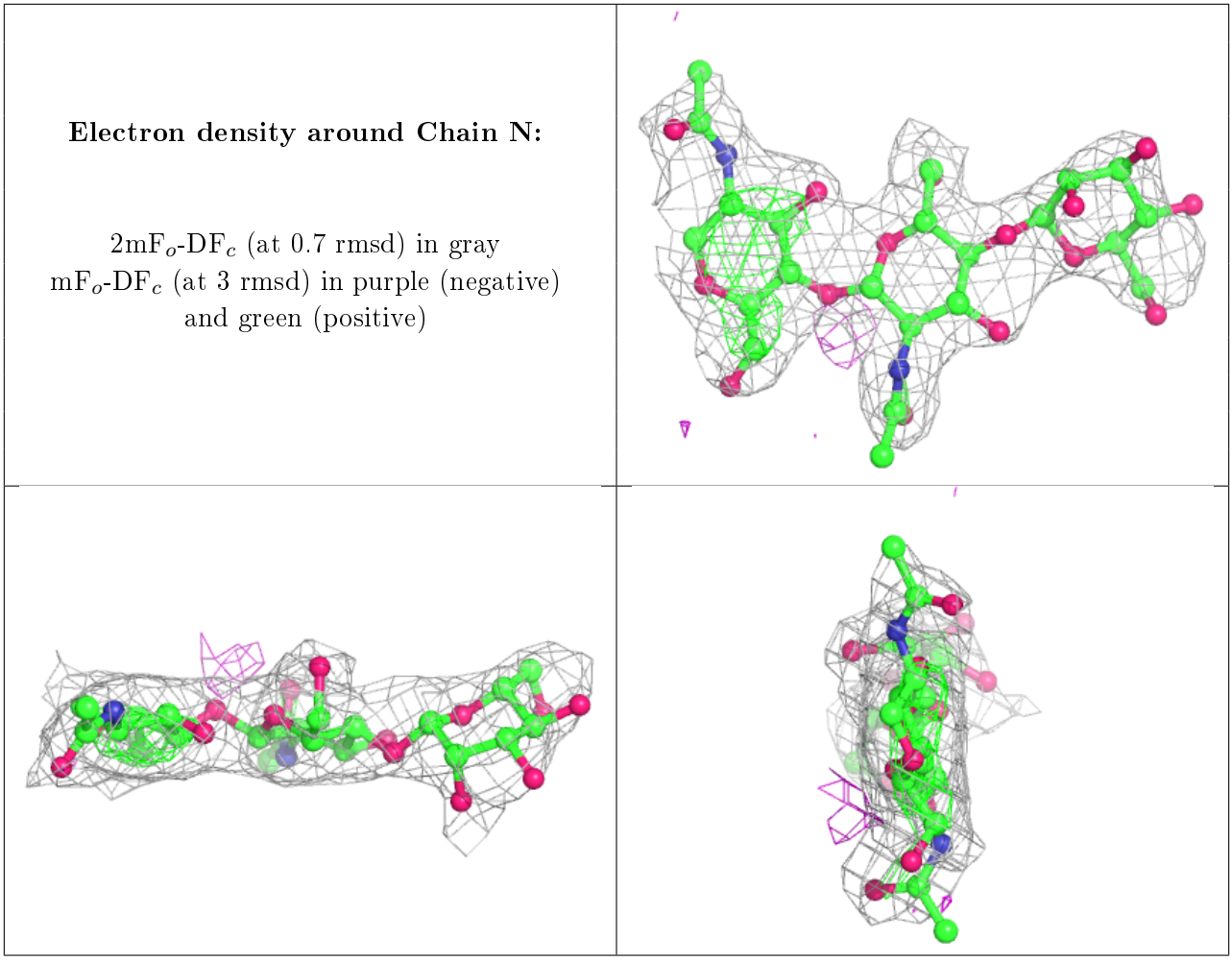
Electron density around Chain H:

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



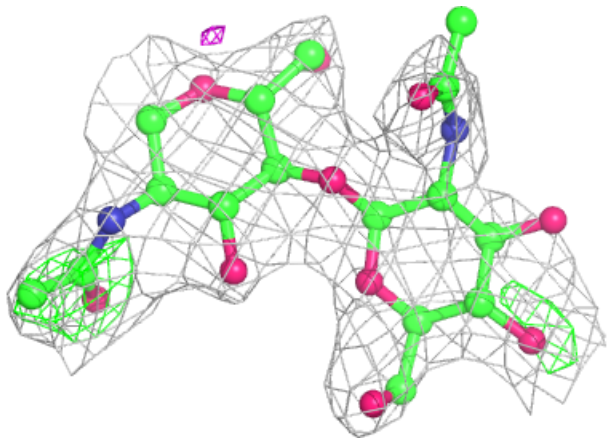
Electron density around Chain N:

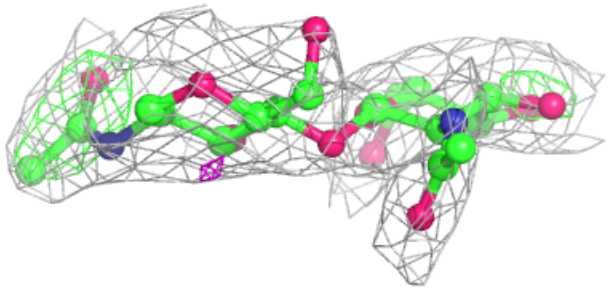
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

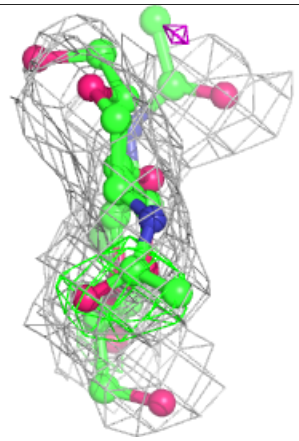


Electron density around Chain F:

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

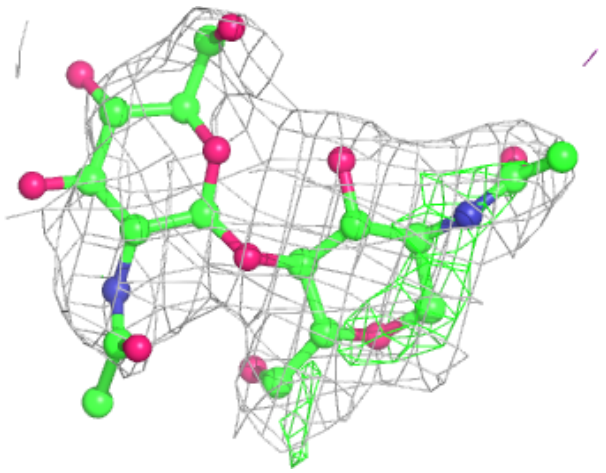


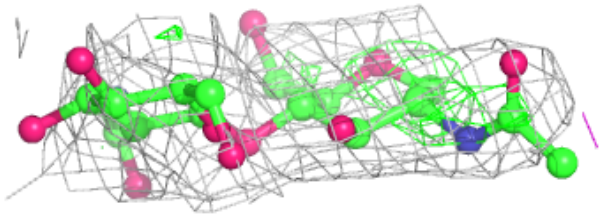


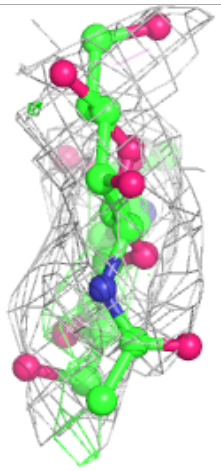


Electron density around Chain G:

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

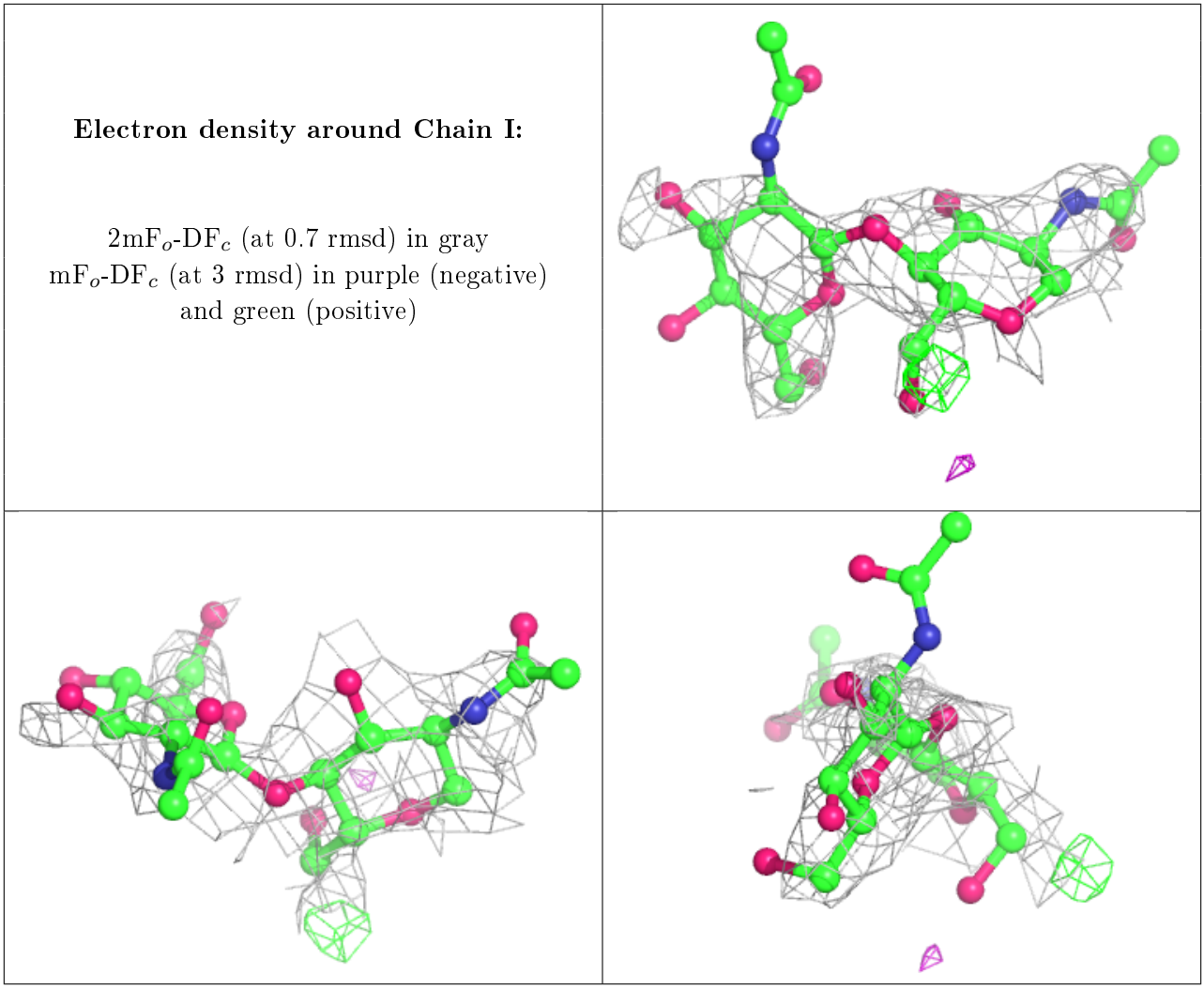






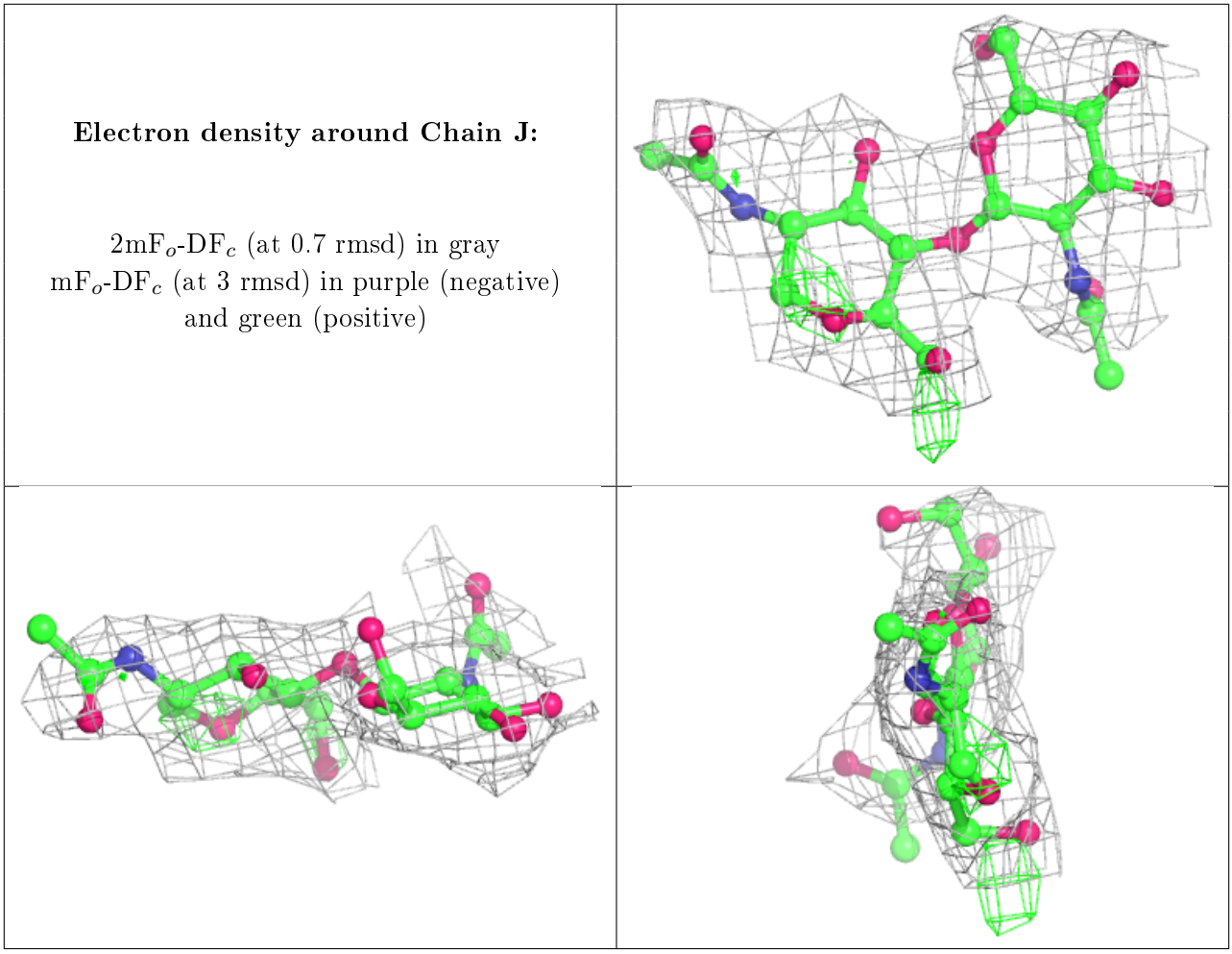
Electron density around Chain I:

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



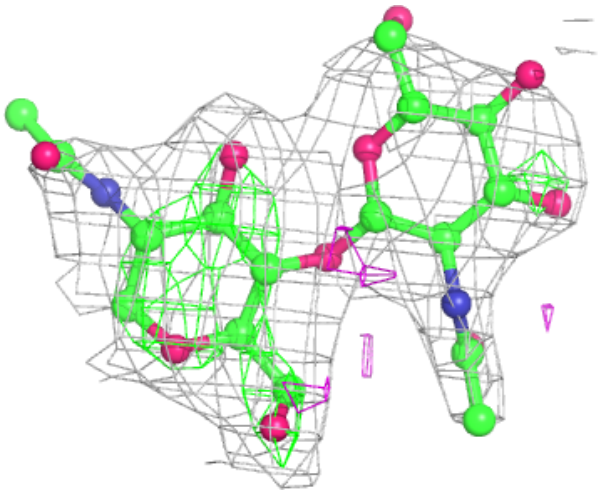
Electron density around Chain J:

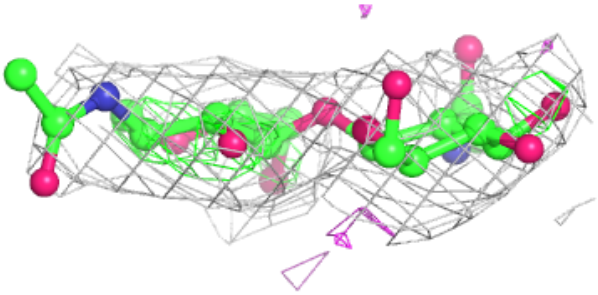
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

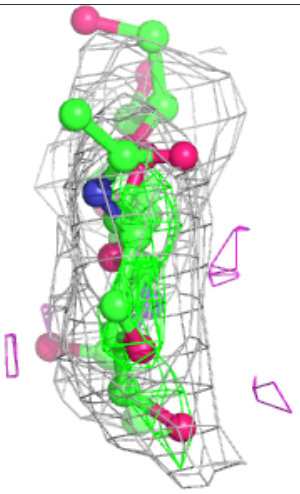


Electron density around Chain K:

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

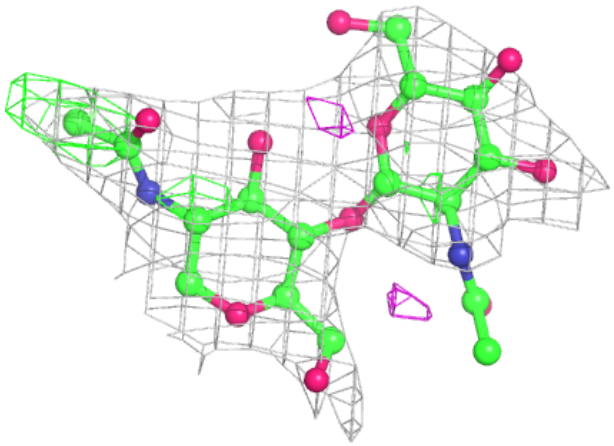


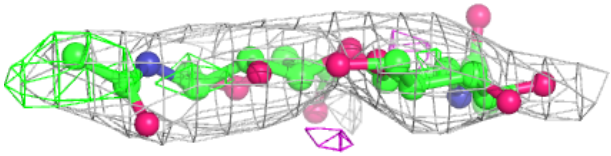


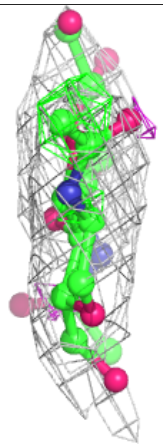


Electron density around Chain L:

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

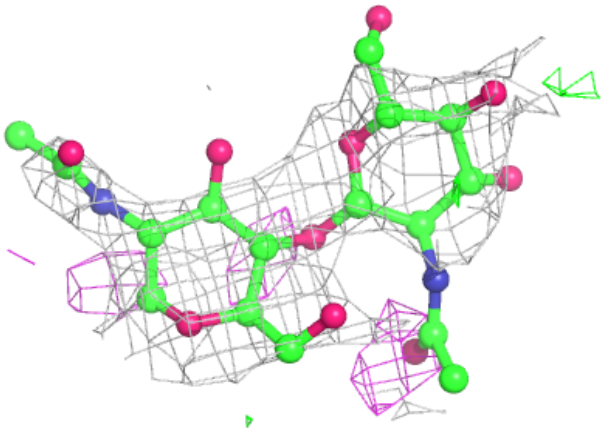


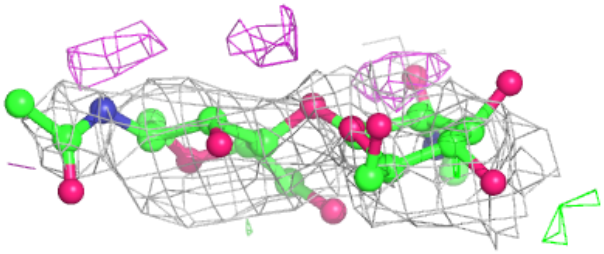


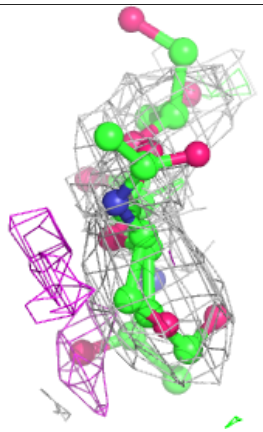


Electron density around Chain O:

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

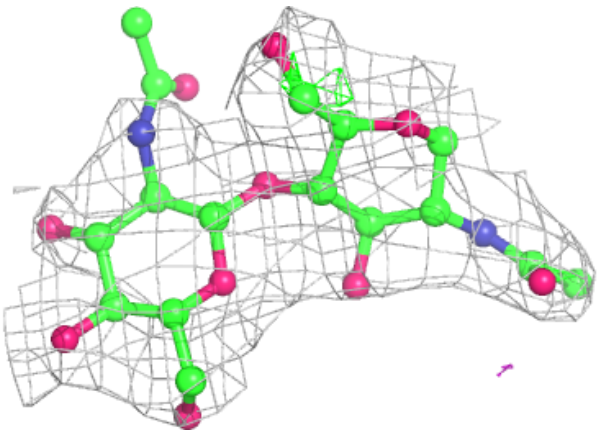


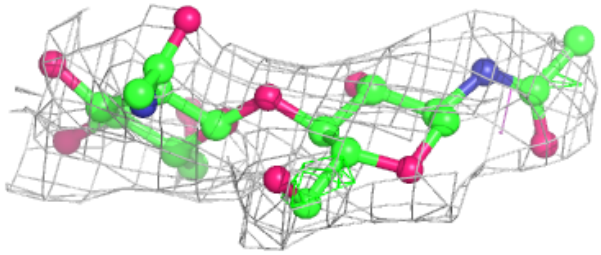


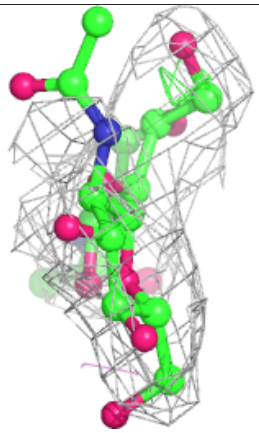


Electron density around Chain P:

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

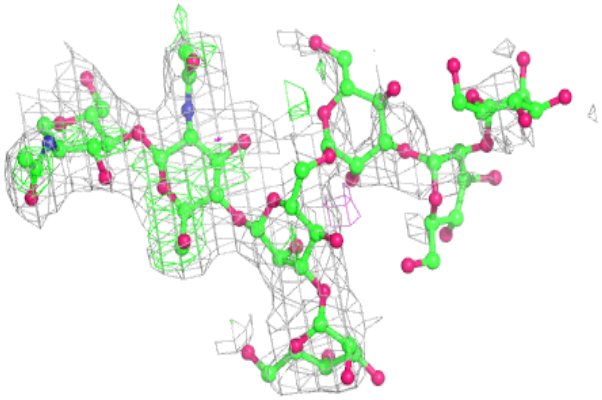


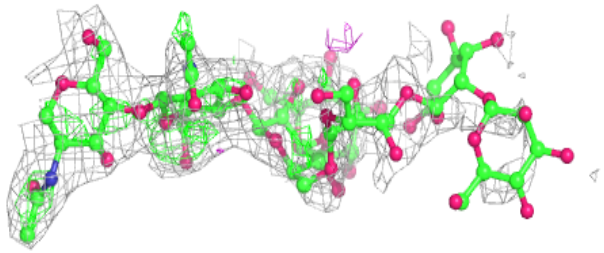


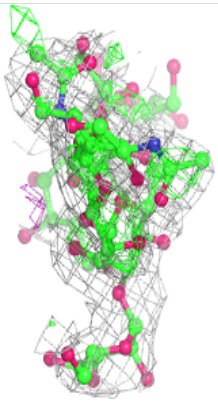


Electron density around Chain M:

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







6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	D	900	14/15	0.70	0.47	159,166,173,173	0
5	NAG	B	900	14/15	0.80	0.29	156,165,172,172	0
5	NAG	A	900	14/15	0.80	0.25	152,159,164,164	0

6.5 Other polymers

There are no such residues in this entry.