Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 04:06 PM EST

PDB ID	:	8GK6
Title	:	Crystal structure of extracellular domain of CNNM4 from Echinococcus granulosus
Authors	:	Shahsavan, A.; Gehring, K.
Deposited on	:	2023-03-17
Resolution	:	2.70 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

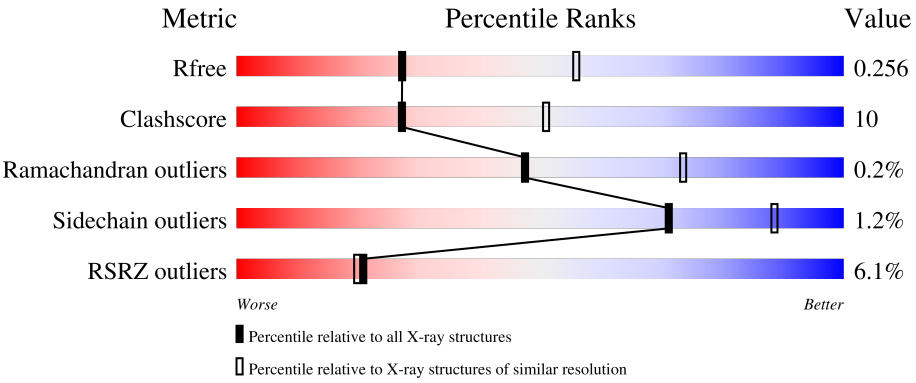
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	139	4% 76% 17% 7%
1	B	139	5% 76% 17% • 6%
1	C	139	6% 75% 17% • 7%
1	D	139	3% 65% 27% 8%
1	E	139	4% 68% 23% • 8%

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Mol	Chain	Length	Quality of chain
1	F	139	4% 70% 22% 8%
1	G	139	5% 75% 17% 8%
1	H	139	14% 67% 24% 8%
2	I	2	50% 50%
3	J	2	50% 50%
3	L	2	50% 50%
3	M	2	50% 50%
4	K	3	33% 67%
5	N	5	20% 80%

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
5	BMA	N	3	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16479 atoms, of which 8094 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 Metal transporter CNNM4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	129	Total	C	H	N	O	S	0	0	0
			1999	654	988	163	192	2			
1	B	130	Total	C	H	N	O	S	0	0	0
			2013	658	995	164	194	2			
1	C	129	Total	C	H	N	O	S	0	0	0
			2003	655	990	163	193	2			
1	D	128	Total	C	H	N	O	S	0	0	0
			1988	651	983	162	190	2			
1	E	128	Total	C	H	N	O	S	0	0	0
			1988	651	983	162	190	2			
1	F	128	Total	C	H	N	O	S	0	0	0
			1987	651	982	162	190	2			
1	H	128	Total	C	H	N	O	S	0	0	0
			1986	651	981	162	190	2			
1	G	128	Total	C	H	N	O	S	0	0	0
			1988	651	983	162	190	2			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ASP	-	expression tag	UNP W6USS8
A	16	ARG	-	expression tag	UNP W6USS8
A	17	HIS	-	expression tag	UNP W6USS8
A	18	HIS	-	expression tag	UNP W6USS8
A	19	HIS	-	expression tag	UNP W6USS8
A	20	HIS	-	expression tag	UNP W6USS8
A	21	HIS	-	expression tag	UNP W6USS8
A	22	HIS	-	expression tag	UNP W6USS8
A	23	GLY	-	expression tag	UNP W6USS8
A	24	SER	-	expression tag	UNP W6USS8
B	15	ASP	-	expression tag	UNP W6USS8
B	16	ARG	-	expression tag	UNP W6USS8
B	17	HIS	-	expression tag	UNP W6USS8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	18	HIS	-	expression tag	UNP W6USS8
B	19	HIS	-	expression tag	UNP W6USS8
B	20	HIS	-	expression tag	UNP W6USS8
B	21	HIS	-	expression tag	UNP W6USS8
B	22	HIS	-	expression tag	UNP W6USS8
B	23	GLY	-	expression tag	UNP W6USS8
B	24	SER	-	expression tag	UNP W6USS8
C	15	ASP	-	expression tag	UNP W6USS8
C	16	ARG	-	expression tag	UNP W6USS8
C	17	HIS	-	expression tag	UNP W6USS8
C	18	HIS	-	expression tag	UNP W6USS8
C	19	HIS	-	expression tag	UNP W6USS8
C	20	HIS	-	expression tag	UNP W6USS8
C	21	HIS	-	expression tag	UNP W6USS8
C	22	HIS	-	expression tag	UNP W6USS8
C	23	GLY	-	expression tag	UNP W6USS8
C	24	SER	-	expression tag	UNP W6USS8
D	15	ASP	-	expression tag	UNP W6USS8
D	16	ARG	-	expression tag	UNP W6USS8
D	17	HIS	-	expression tag	UNP W6USS8
D	18	HIS	-	expression tag	UNP W6USS8
D	19	HIS	-	expression tag	UNP W6USS8
D	20	HIS	-	expression tag	UNP W6USS8
D	21	HIS	-	expression tag	UNP W6USS8
D	22	HIS	-	expression tag	UNP W6USS8
D	23	GLY	-	expression tag	UNP W6USS8
D	24	SER	-	expression tag	UNP W6USS8
E	15	ASP	-	expression tag	UNP W6USS8
E	16	ARG	-	expression tag	UNP W6USS8
E	17	HIS	-	expression tag	UNP W6USS8
E	18	HIS	-	expression tag	UNP W6USS8
E	19	HIS	-	expression tag	UNP W6USS8
E	20	HIS	-	expression tag	UNP W6USS8
E	21	HIS	-	expression tag	UNP W6USS8
E	22	HIS	-	expression tag	UNP W6USS8
E	23	GLY	-	expression tag	UNP W6USS8
E	24	SER	-	expression tag	UNP W6USS8
F	15	ASP	-	expression tag	UNP W6USS8
F	16	ARG	-	expression tag	UNP W6USS8
F	17	HIS	-	expression tag	UNP W6USS8
F	18	HIS	-	expression tag	UNP W6USS8
F	19	HIS	-	expression tag	UNP W6USS8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	20	HIS	-	expression tag	UNP W6USS8
F	21	HIS	-	expression tag	UNP W6USS8
F	22	HIS	-	expression tag	UNP W6USS8
F	23	GLY	-	expression tag	UNP W6USS8
F	24	SER	-	expression tag	UNP W6USS8
H	15	ASP	-	expression tag	UNP W6USS8
H	16	ARG	-	expression tag	UNP W6USS8
H	17	HIS	-	expression tag	UNP W6USS8
H	18	HIS	-	expression tag	UNP W6USS8
H	19	HIS	-	expression tag	UNP W6USS8
H	20	HIS	-	expression tag	UNP W6USS8
H	21	HIS	-	expression tag	UNP W6USS8
H	22	HIS	-	expression tag	UNP W6USS8
H	23	GLY	-	expression tag	UNP W6USS8
H	24	SER	-	expression tag	UNP W6USS8
G	15	ASP	-	expression tag	UNP W6USS8
G	16	ARG	-	expression tag	UNP W6USS8
G	17	HIS	-	expression tag	UNP W6USS8
G	18	HIS	-	expression tag	UNP W6USS8
G	19	HIS	-	expression tag	UNP W6USS8
G	20	HIS	-	expression tag	UNP W6USS8
G	21	HIS	-	expression tag	UNP W6USS8
G	22	HIS	-	expression tag	UNP W6USS8
G	23	GLY	-	expression tag	UNP W6USS8
G	24	SER	-	expression tag	UNP W6USS8

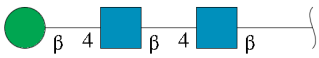
- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	2	Total	C	H	N	O	0	0	0
			39	14	15	1	9			

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

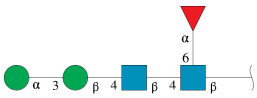
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	2	Total	C	H	N	O	0	0	0
			51	16	23	2	10			
3	L	2	Total	C	H	N	O	0	0	0
			51	16	23	2	10			
3	M	2	Total	C	H	N	O	0	0	0
			51	16	23	2	10			

- Molecule 4 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.



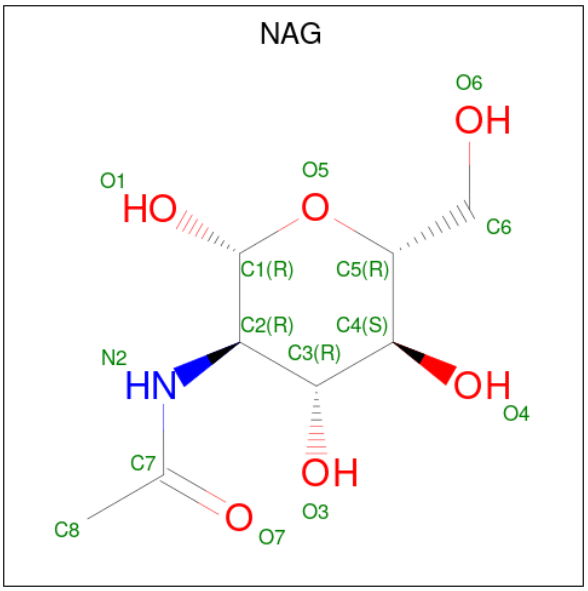
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	3	Total	C	H	N	O	0	0	0
			67	22	28	2	15			

- Molecule 5 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-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	N	5	Total	C	H	N	O	0	0	0
			97	34	37	2	24			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C H N O 26 8 12 1 5	0	0
6	E	1	Total C H N O 26 8 12 1 5	0	0
6	E	1	Total C H N O 26 8 12 1 5	0	0
6	F	1	Total C H N O 26 8 12 1 5	0	0
6	H	1	Total C H N O 26 8 12 1 5	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	7	Total O 7 7	0	0
7	B	8	Total O 8 8	0	0
7	C	7	Total O 7 7	0	0
7	D	6	Total O 6 6	0	0
7	E	5	Total O 5 5	0	0
7	F	3	Total O 3 3	0	0
7	H	3	Total O 3 3	0	0

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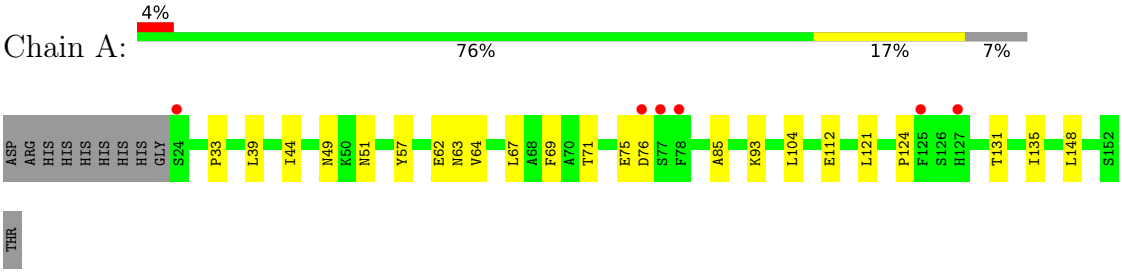
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	2	Total O 2 2	0	0

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.

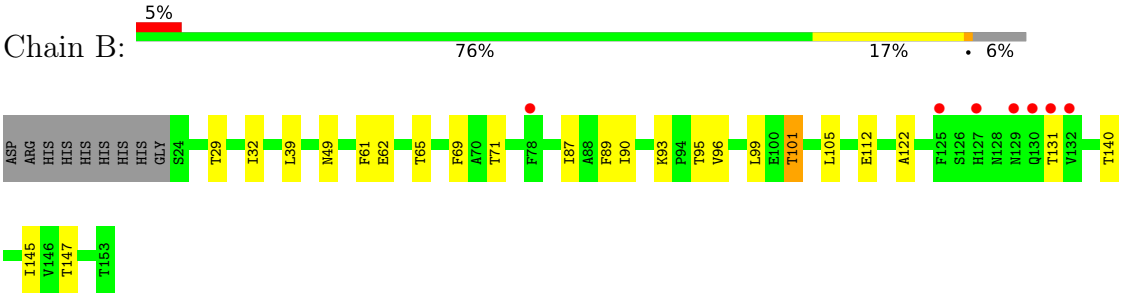
• Molecule 1: Metal transporter CNNM4

Chain A:



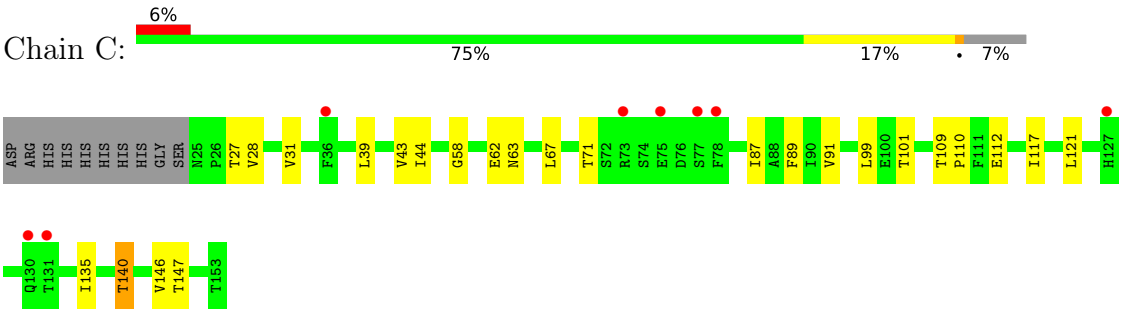
• Molecule 1: Metal transporter CNNM4

Chain B:



• Molecule 1: Metal transporter CNNM4

Chain C:

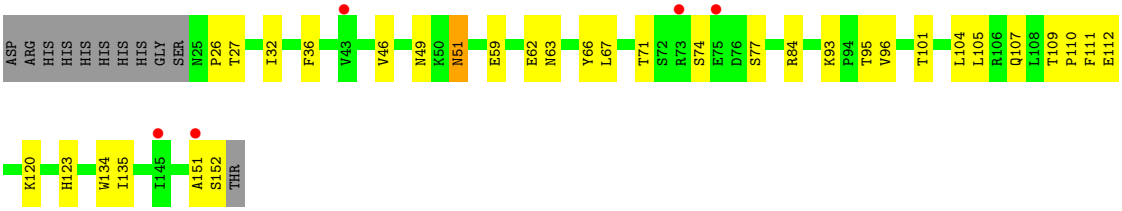


• Molecule 1: Metal transporter CNNM4

Chain D:

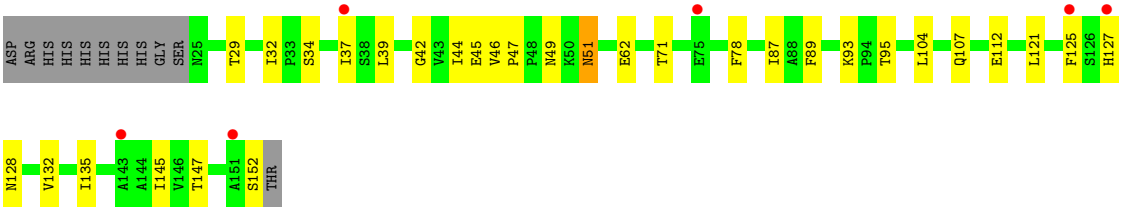
• Molecule 1: Metal transporter CNNM4

Chain E:



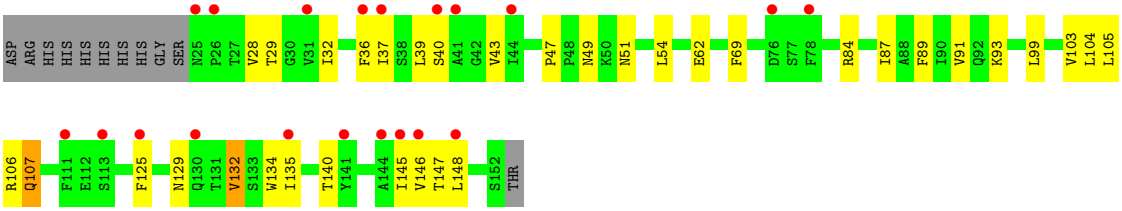
• Molecule 1: Metal transporter CNNM4

Chain F:



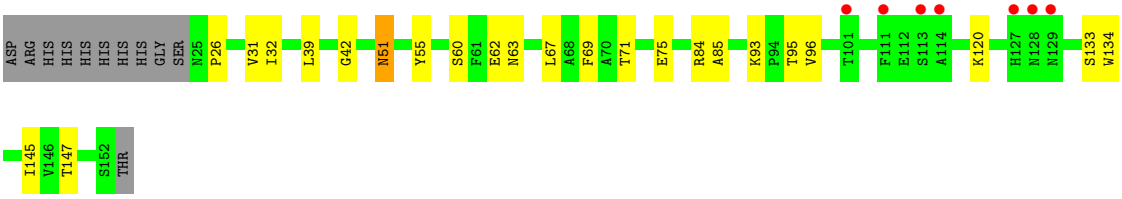
• Molecule 1: Metal transporter CNNM4

Chain H:



• Molecule 1: Metal transporter CNNM4

Chain G:



• Molecule 2: alpha-L-fucopyranose-(1-6)-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

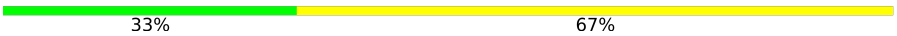
Chain L:

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

Chain M:

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

Chain K:



• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.34Å 120.76Å 95.25Å 90.00° 98.09° 90.00°	Depositor
Resolution (Å)	46.64 – 2.70 46.64 – 2.70	Depositor EDS
% Data completeness (in resolution range)	68.2 (46.64-2.70) 81.9 (46.64-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.197 , 0.253 0.202 , 0.256	Depositor DCC
R_{free} test set	1979 reflections (6.78%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	16479	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: FUC, MAN, BMA, NAG

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	0.34	0/1040	0.56	0/1426
1	B	0.30	0/1047	0.55	0/1436
1	C	0.30	0/1042	0.55	0/1428
1	D	0.31	0/1034	0.56	0/1418
1	E	0.32	0/1034	0.56	0/1418
1	F	0.30	0/1034	0.54	0/1418
1	G	0.28	0/1034	0.52	0/1418
1	H	0.33	0/1034	0.57	0/1418
All	All	0.31	0/8299	0.55	0/11380

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1011	988	987	20	0
1	B	1018	995	995	16	0
1	C	1013	990	989	20	0
1	D	1005	983	982	29	0
1	E	1005	983	981	25	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1005	982	982	26	0
1	G	1005	983	983	15	1
1	H	1005	981	980	25	0
2	I	24	15	22	1	0
3	J	28	23	25	3	0
3	L	28	23	25	4	0
3	M	28	23	25	2	0
4	K	39	28	34	3	0
5	N	60	37	52	7	0
6	D	14	12	13	1	0
6	E	28	24	26	4	0
6	F	14	12	13	1	0
6	H	14	12	13	1	0
7	A	7	0	0	0	0
7	B	8	0	0	0	0
7	C	7	0	0	0	0
7	D	6	0	0	0	0
7	E	5	0	0	0	0
7	F	3	0	0	0	0
7	G	2	0	0	0	0
7	H	3	0	0	0	0
All	All	8385	8094	8127	167	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (167) 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:G:39:LEU:HD11	1:G:145:ILE:HD13	1.50	0.92
1:G:62:GLU:O	1:G:93:LYS:NZ	2.09	0.84
5:N:2:NAG:O3	5:N:3:BMA:O2	1.92	0.81
1:E:51:ASN:OD1	6:E:201:NAG:H2	1.85	0.77
1:C:27:THR:HG21	1:C:140:THR:HG23	1.65	0.76
1:F:37:ILE:HD13	1:F:45:GLU:HG2	1.66	0.76
1:D:59:GLU:OE1	1:F:95:THR:HG21	1.87	0.74
1:F:37:ILE:HD11	1:F:46:VAL:C	2.12	0.70
1:C:63:ASN:OD1	4:K:1:NAG:H2	1.91	0.70
1:C:39:LEU:HD13	1:C:44:ILE:HG12	1.74	0.69
1:A:57:TYR:HB2	1:E:32:ILE:HD11	1.75	0.69
1:H:129:ASN:OD1	3:M:1:NAG:H2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ILE:HD11	1:F:34:SER:O	1.95	0.66
1:F:51:ASN:HD22	6:F:201:NAG:C7	2.09	0.65
1:D:63:ASN:OD1	3:L:1:NAG:H2	1.96	0.65
1:B:32:ILE:HD11	1:G:32:ILE:HD13	1.79	0.64
1:E:63:ASN:OD1	6:E:202:NAG:H2	1.97	0.63
5:N:3:BMA:H2	5:N:4:MAN:H5	1.80	0.62
5:N:2:NAG:HO3	5:N:3:BMA:HO2	1.17	0.62
1:F:87:ILE:HD11	1:F:89:PHE:CE1	2.35	0.61
1:E:51:ASN:OD1	6:E:201:NAG:C2	2.47	0.61
1:F:49:ASN:HA	1:F:104:LEU:HD21	1.82	0.61
1:F:37:ILE:CD1	1:F:46:VAL:C	2.68	0.60
1:B:62:GLU:O	1:B:93:LYS:NZ	2.35	0.60
1:A:44:ILE:HB	1:A:148:LEU:HD23	1.83	0.60
1:F:37:ILE:HD11	1:F:47:PRO:N	2.17	0.59
1:C:31:VAL:O	1:H:32:ILE:HD11	2.03	0.59
1:H:49:ASN:HA	1:H:104:LEU:HD21	1.84	0.59
1:H:29:THR:OG1	1:H:140:THR:HG21	2.03	0.58
1:D:55:TYR:CD1	1:D:100:GLU:HG2	2.39	0.58
1:H:54:LEU:HD13	1:H:103:VAL:HG22	1.85	0.58
1:A:63:ASN:OD1	3:J:1:NAG:H2	2.03	0.58
1:C:63:ASN:OD1	4:K:1:NAG:C2	2.46	0.58
1:A:71:THR:HG23	1:A:85:ALA:HB3	1.85	0.57
1:C:39:LEU:HD13	1:C:44:ILE:CG1	2.35	0.57
1:C:87:ILE:HD11	1:C:89:PHE:CE1	2.40	0.56
1:D:27:THR:HG22	1:D:138:THR:HB	1.88	0.56
1:B:71:THR:HG21	1:B:112:GLU:OE2	2.06	0.55
1:D:121:LEU:HD11	1:D:135:ILE:HD13	1.88	0.55
1:F:37:ILE:CD1	1:F:46:VAL:CA	2.85	0.55
1:H:37:ILE:HD12	1:H:37:ILE:N	2.22	0.54
1:H:62:GLU:O	1:H:93:LYS:NZ	2.40	0.54
1:D:63:ASN:OD1	3:L:1:NAG:C2	2.49	0.54
1:A:71:THR:HG21	1:A:112:GLU:OE2	2.07	0.54
1:A:39:LEU:HD23	1:E:36:PHE:O	2.08	0.54
1:F:37:ILE:HD12	1:F:46:VAL:HA	1.90	0.54
1:F:71:THR:HG21	1:F:112:GLU:OE2	2.08	0.53
1:C:27:THR:CG2	1:C:140:THR:HG23	2.38	0.53
1:H:106:ARG:O	1:H:107:GLN:C	2.47	0.53
1:A:121:LEU:HD11	1:A:135:ILE:HD13	1.91	0.53
1:E:84:ARG:HD2	1:E:134:TRP:CD2	2.43	0.53
1:F:121:LEU:HD11	1:F:135:ILE:HD13	1.89	0.53
1:H:43:VAL:HG22	1:H:147:THR:OG1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:ASN:HB2	6:H:201:NAG:N2	2.25	0.52
1:E:27:THR:HG22	1:E:59:GLU:O	2.07	0.52
1:E:26:PRO:HG2	1:E:135:ILE:HD11	1.91	0.52
1:B:49:ASN:HB3	1:D:111:PHE:HE2	1.73	0.52
1:E:46:VAL:HG21	1:E:105:LEU:HD12	1.91	0.52
1:E:67:LEU:HD22	1:E:101:THR:HG21	1.91	0.52
1:A:49:ASN:HA	1:A:104:LEU:HD21	1.91	0.51
1:C:71:THR:HG21	1:C:112:GLU:OE2	2.10	0.51
1:H:84:ARG:HD2	1:H:134:TRP:CD2	2.45	0.51
1:A:62:GLU:HB3	3:J:1:NAG:H82	1.92	0.51
1:C:28:VAL:HG12	1:C:146:VAL:HG12	1.93	0.51
1:E:107:GLN:NE2	1:E:152:SER:O	2.44	0.51
1:F:37:ILE:HD12	1:F:46:VAL:CA	2.41	0.51
5:N:2:NAG:O3	5:N:3:BMA:C2	2.58	0.51
1:D:33:PRO:HG3	1:D:44:ILE:HG21	1.93	0.51
1:C:62:GLU:HG2	4:K:1:NAG:H82	1.93	0.51
1:A:64:VAL:O	1:A:93:LYS:NZ	2.40	0.50
1:G:67:LEU:HD21	1:G:69:PHE:CZ	2.47	0.50
1:F:39:LEU:HD13	1:F:44:ILE:HG12	1.93	0.49
1:D:97:TYR:OH	1:F:29:THR:OG1	2.12	0.49
1:E:67:LEU:CD2	1:E:101:THR:HG21	2.43	0.49
1:F:37:ILE:HD12	1:F:45:GLU:O	2.13	0.49
1:A:75:GLU:O	1:D:128:ASN:OD1	2.30	0.49
1:D:51:ASN:OD1	6:D:201:NAG:C1	2.61	0.49
1:D:62:GLU:OE2	3:L:1:NAG:N2	2.43	0.49
1:A:57:TYR:CB	1:E:32:ILE:HD11	2.42	0.49
1:D:65:THR:CG2	1:D:122:ALA:HB2	2.43	0.48
1:G:51:ASN:OD1	5:N:1:NAG:C1	2.61	0.48
1:D:55:TYR:HD1	1:D:100:GLU:HG2	1.78	0.48
1:D:57:TYR:CD2	1:F:32:ILE:HD11	2.48	0.48
1:G:71:THR:HG23	1:G:85:ALA:CB	2.43	0.48
1:A:124:PRO:HB2	1:A:131:THR:OG1	2.14	0.48
1:D:64:VAL:O	1:D:93:LYS:NZ	2.41	0.48
1:B:93:LYS:HG2	1:B:99:LEU:HD23	1.96	0.48
1:B:71:THR:HG21	1:B:112:GLU:CD	2.34	0.47
1:G:42:GLY:HA2	1:G:145:ILE:HG12	1.96	0.47
1:B:69:PHE:CE2	1:B:105:LEU:HD21	2.49	0.47
1:H:54:LEU:HD21	1:H:148:LEU:HD11	1.97	0.47
1:E:95:THR:HG22	1:E:96:VAL:N	2.30	0.47
1:H:87:ILE:HD11	1:H:89:PHE:CE1	2.49	0.47
1:F:107:GLN:NE2	1:F:152:SER:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:84:ARG:HD3	1:G:134:TRP:CD2	2.49	0.47
1:B:90:ILE:O	1:B:101:THR:HG23	2.14	0.47
1:E:49:ASN:HA	1:E:104:LEU:HD21	1.97	0.47
1:A:51:ASN:OD1	2:I:1:NAG:C1	2.63	0.46
1:H:39:LEU:HD11	1:H:145:ILE:HD13	1.97	0.46
1:G:26:PRO:HA	1:G:60:SER:HB2	1.98	0.46
1:A:76:ASP:CG	1:D:79:SER:HB3	2.36	0.46
1:E:74:SER:O	1:E:77:SER:OG	2.32	0.46
5:N:2:NAG:C3	5:N:3:BMA:C2	2.94	0.46
1:C:121:LEU:HD11	1:C:135:ILE:HD13	1.98	0.46
1:E:63:ASN:OD1	6:E:202:NAG:C2	2.54	0.46
1:E:84:ARG:HD2	1:E:134:TRP:CE2	2.51	0.45
1:G:32:ILE:HB	1:G:55:TYR:HB2	1.98	0.45
1:C:109:THR:HB	1:C:110:PRO:HD2	1.97	0.45
1:F:78:PHE:O	1:F:135:ILE:HA	2.16	0.45
1:E:71:THR:HG21	1:E:112:GLU:OE2	2.17	0.45
1:H:54:LEU:CD1	1:H:103:VAL:HG22	2.47	0.45
1:D:62:GLU:HG2	3:L:1:NAG:H82	1.99	0.44
1:C:91:VAL:CG2	1:C:99:LEU:HB3	2.47	0.44
1:D:87:ILE:HD11	1:D:89:PHE:CE1	2.53	0.44
1:G:62:GLU:HG3	1:G:63:ASN:N	2.32	0.44
1:C:91:VAL:HG21	1:C:99:LEU:HB3	2.00	0.44
1:C:27:THR:O	1:C:58:GLY:HA3	2.18	0.44
1:D:61:PHE:CD2	1:D:99:LEU:HG	2.53	0.44
1:B:61:PHE:CD2	1:B:99:LEU:HG	2.52	0.44
1:C:67:LEU:CD1	1:C:117:ILE:HG23	2.48	0.44
1:B:32:ILE:HD11	1:G:31:VAL:O	2.18	0.43
1:E:66:TYR:HB2	1:E:120:LYS:HB3	2.00	0.43
1:D:61:PHE:O	1:D:93:LYS:HE2	2.18	0.43
1:E:111:PHE:N	1:E:111:PHE:CD1	2.86	0.43
1:H:28:VAL:HG12	1:H:146:VAL:HG12	2.00	0.43
1:H:51:ASN:N	1:H:104:LEU:HD12	2.32	0.43
1:G:95:THR:HG22	1:G:96:VAL:N	2.34	0.43
1:B:87:ILE:HD11	1:B:89:PHE:CE1	2.53	0.43
1:B:65:THR:CG2	1:B:122:ALA:HB2	2.48	0.43
1:H:37:ILE:HD11	1:H:47:PRO:HD3	2.01	0.43
5:N:3:BMA:H2	5:N:4:MAN:C5	2.47	0.43
1:B:39:LEU:HD11	1:B:145:ILE:HG12	2.01	0.43
1:A:33:PRO:HG2	1:A:44:ILE:HG21	2.01	0.43
1:A:63:ASN:OD1	3:J:1:NAG:C2	2.60	0.43
1:D:44:ILE:HB	1:D:148:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:THR:HB	1:E:110:PRO:HD2	2.01	0.43
1:B:29:THR:HA	1:B:140:THR:OG1	2.19	0.43
1:C:39:LEU:HB2	1:H:36:PHE:CE2	2.54	0.43
1:C:39:LEU:HD12	1:C:43:VAL:O	2.18	0.42
1:H:69:PHE:CD2	1:H:105:LEU:HD21	2.54	0.42
1:F:42:GLY:HA2	1:F:145:ILE:HG12	1.99	0.42
1:H:91:VAL:CG2	1:H:99:LEU:HB3	2.49	0.42
1:E:107:GLN:CG	1:E:151:ALA:O	2.68	0.42
1:B:131:THR:HG21	1:D:124:PRO:HG3	2.01	0.42
1:G:95:THR:HG22	1:G:96:VAL:H	1.84	0.42
1:F:78:PHE:CE2	1:F:125:PHE:CE2	3.08	0.42
1:F:125:PHE:CZ	1:F:132:VAL:CG2	3.02	0.42
1:D:26:PRO:HD2	1:D:135:ILE:HD11	2.01	0.41
1:D:49:ASN:HA	1:D:104:LEU:HD21	2.01	0.41
1:F:39:LEU:HD11	1:F:145:ILE:HD13	2.02	0.41
1:H:125:PHE:CZ	1:H:132:VAL:HG23	2.55	0.41
1:G:120:LYS:HA	1:G:133:SER:O	2.20	0.41
1:H:125:PHE:HZ	1:H:135:ILE:CG2	2.33	0.41
1:A:71:THR:HG23	1:A:85:ALA:CB	2.50	0.41
1:C:67:LEU:HD22	1:C:101:THR:HG21	2.03	0.41
1:F:62:GLU:O	1:F:93:LYS:NZ	2.54	0.41
1:B:96:VAL:O	1:B:96:VAL:HG22	2.21	0.41
1:D:71:THR:HG21	1:D:112:GLU:OE2	2.21	0.41
1:D:81:GLU:HG2	1:D:132:VAL:HG13	2.03	0.41
1:H:129:ASN:OD1	3:M:1:NAG:C2	2.51	0.41
1:A:64:VAL:O	1:A:93:LYS:CE	2.69	0.41
1:E:71:THR:HG21	1:E:112:GLU:CD	2.41	0.40
1:H:39:LEU:HD23	1:H:40:SER:N	2.36	0.40
1:A:67:LEU:HD21	1:A:69:PHE:CZ	2.55	0.40
1:F:127:HIS:O	1:F:128:ASN:OD1	2.40	0.40
1:D:69:PHE:CE2	1:D:105:LEU:HD21	2.56	0.40
1:E:62:GLU:O	1:E:93:LYS:NZ	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:TYR:OH	1:G:75:GLU:OE2[1_655]	1.96	0.24

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	127/139 (91%)	121 (95%)	6 (5%)	0	100	100
1	B	128/139 (92%)	122 (95%)	6 (5%)	0	100	100
1	C	127/139 (91%)	121 (95%)	6 (5%)	0	100	100
1	D	126/139 (91%)	121 (96%)	5 (4%)	0	100	100
1	E	126/139 (91%)	119 (94%)	6 (5%)	1 (1%)	19	43
1	F	126/139 (91%)	121 (96%)	5 (4%)	0	100	100
1	G	126/139 (91%)	120 (95%)	6 (5%)	0	100	100
1	H	126/139 (91%)	123 (98%)	2 (2%)	1 (1%)	19	43
All	All	1012/1112 (91%)	968 (96%)	42 (4%)	2 (0%)	47	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	107	GLN
1	E	123	HIS

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	115/124 (93%)	115 (100%)	0	100	100
1	B	116/124 (94%)	113 (97%)	3 (3%)	46	75
1	C	115/124 (93%)	113 (98%)	2 (2%)	60	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	114/124 (92%)	114 (100%)	0	100 100
1	E	114/124 (92%)	113 (99%)	1 (1%)	78 92
1	F	114/124 (92%)	112 (98%)	2 (2%)	59 83
1	G	114/124 (92%)	112 (98%)	2 (2%)	59 83
1	H	114/124 (92%)	113 (99%)	1 (1%)	78 92
All	All	916/992 (92%)	905 (99%)	11 (1%)	71 88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	95	THR
1	B	101	THR
1	B	147	THR
1	C	140	THR
1	C	147	THR
1	E	51	ASN
1	F	51	ASN
1	F	147	THR
1	H	132	VAL
1	G	51	ASN
1	G	147	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	127	HIS

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)

16 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	I	1	2	14,14,15	0.74	1 (7%)	17,19,21	0.57	0
2	FUC	I	2	2	10,10,11	0.61	0	14,14,16	0.83	0
3	NAG	J	1	3,1	14,14,15	0.34	0	17,19,21	0.64	0
3	NAG	J	2	3	14,14,15	0.59	0	17,19,21	0.61	0
4	NAG	K	1	4,1	14,14,15	0.44	0	17,19,21	0.61	0
4	NAG	K	2	4	14,14,15	0.64	1 (7%)	17,19,21	0.58	0
4	BMA	K	3	4	11,11,12	0.63	0	15,15,17	0.74	0
3	NAG	L	1	3,1	14,14,15	0.51	0	17,19,21	0.62	0
3	NAG	L	2	3	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	M	1	3,1	14,14,15	0.38	0	17,19,21	0.62	0
3	NAG	M	2	3	14,14,15	0.26	0	17,19,21	0.54	0
5	NAG	N	1	5	14,14,15	0.82	1 (7%)	17,19,21	0.71	0
5	NAG	N	2	5	14,14,15	0.87	1 (7%)	17,19,21	1.10	1 (5%)
5	BMA	N	3	5	11,11,12	1.31	2 (18%)	15,15,17	1.20	3 (20%)
5	MAN	N	4	5	11,11,12	1.60	3 (27%)	15,15,17	2.27	4 (26%)
5	FUC	N	5	5	10,10,11	0.66	0	14,14,16	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	I	1	2	-	0/6/23/26	0/1/1/1
2	FUC	I	2	2	-	-	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	2	NAG	O5-C1	-3.17	1.38	1.43
5	N	4	MAN	O5-C1	3.13	1.48	1.43
5	N	4	MAN	C1-C2	2.92	1.58	1.52
5	N	1	NAG	O5-C1	-2.90	1.39	1.43
2	I	1	NAG	O5-C1	-2.66	1.39	1.43
5	N	4	MAN	O5-C5	2.65	1.48	1.43
5	N	3	BMA	C4-C3	2.09	1.57	1.52
5	N	3	BMA	C4-C5	2.04	1.57	1.53
4	K	2	NAG	C1-C2	2.01	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	4	MAN	C1-O5-C5	6.88	121.52	112.19
5	N	4	MAN	O5-C1-C2	2.96	115.34	110.77
5	N	2	NAG	O4-C4-C5	-2.87	102.16	109.30
5	N	3	BMA	O5-C1-C2	-2.35	107.14	110.77
5	N	4	MAN	C3-C4-C5	-2.23	106.26	110.24
5	N	3	BMA	O2-C2-C3	-2.21	105.71	110.14
5	N	4	MAN	O2-C2-C3	-2.19	105.76	110.14
5	N	3	BMA	C1-O5-C5	-2.14	109.29	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	N	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	J	1	NAG	C4-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
5	N	3	BMA	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
5	N	3	BMA	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6

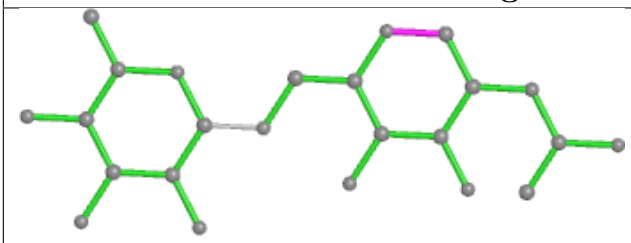
There are no ring outliers.

9 monomers are involved in 20 short contacts:

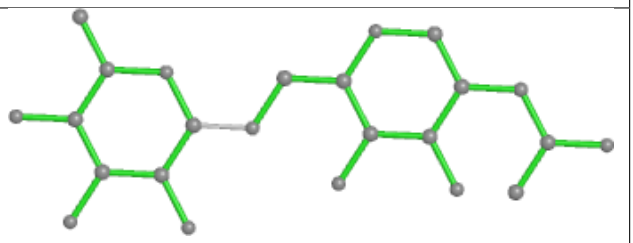
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	NAG	3	0
3	J	1	NAG	3	0
5	N	4	MAN	2	0
5	N	3	BMA	6	0
5	N	2	NAG	4	0
3	M	1	NAG	2	0
2	I	1	NAG	1	0
3	L	1	NAG	4	0
5	N	1	NAG	1	0

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

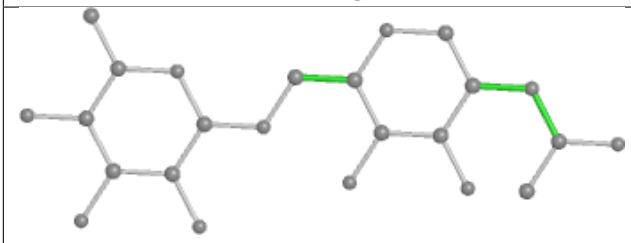
Oligosaccharide Chain I



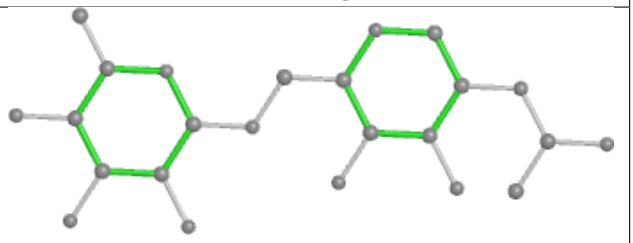
Bond lengths



Bond angles

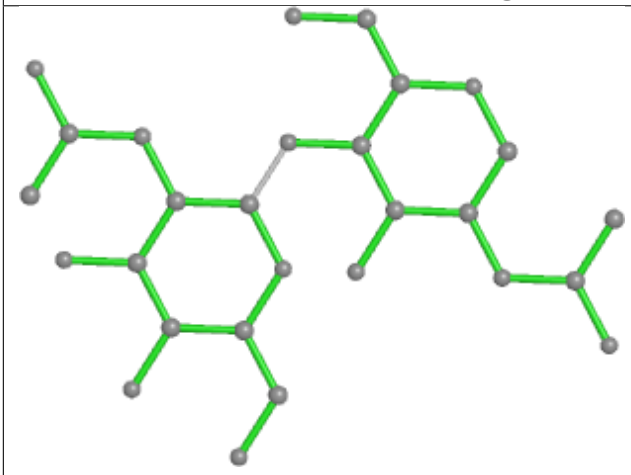


Torsions

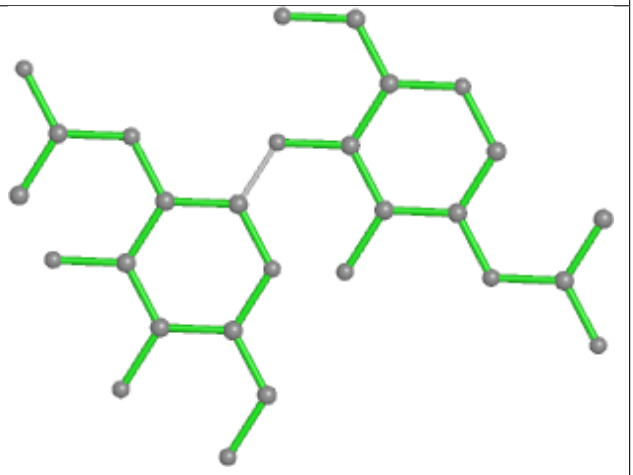


Rings

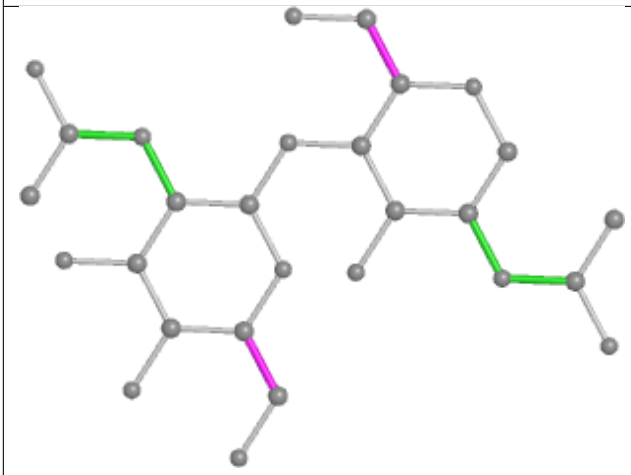
Oligosaccharide Chain J



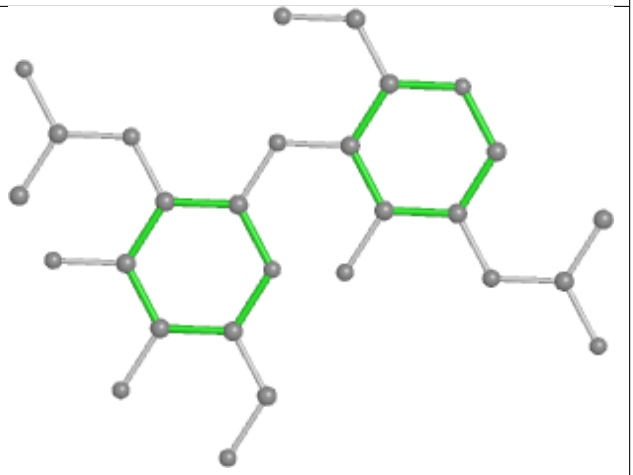
Bond lengths



Bond angles

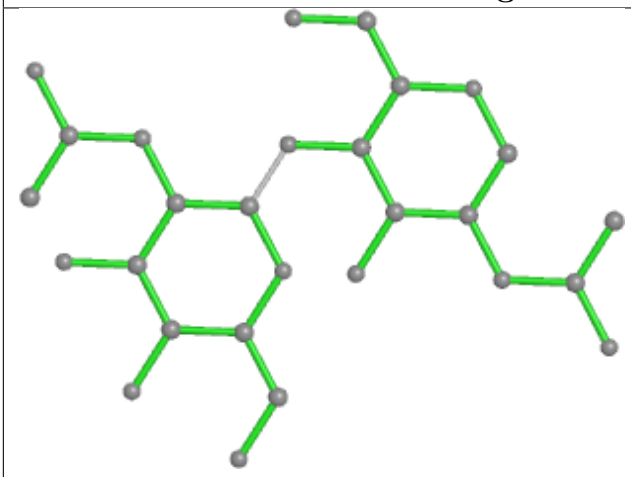


Torsions

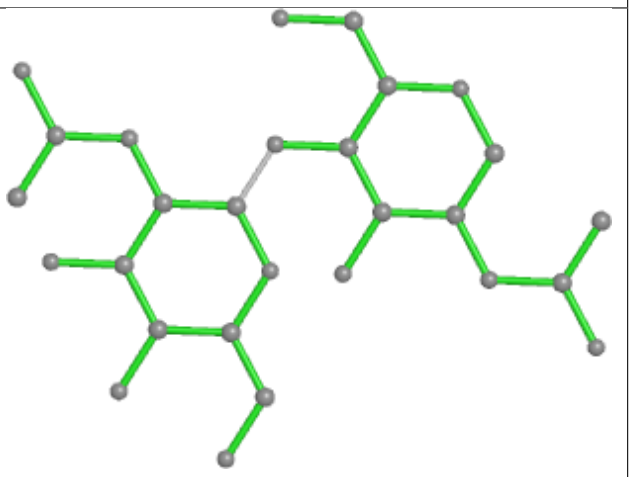


Rings

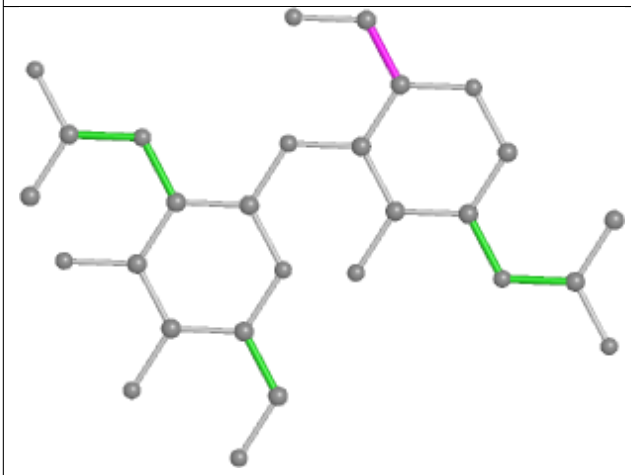
Oligosaccharide Chain L



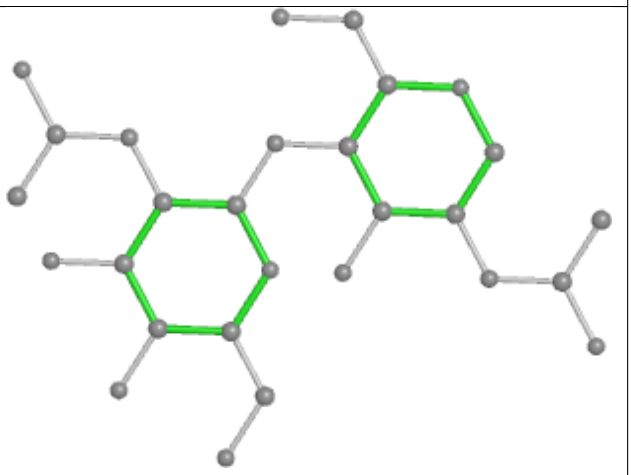
Bond lengths



Bond angles

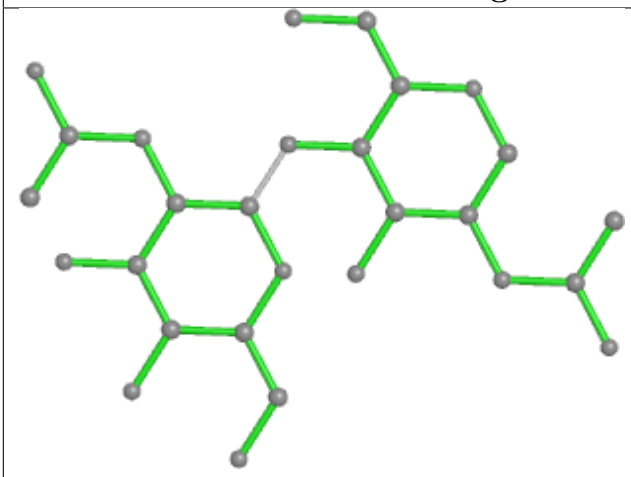


Torsions

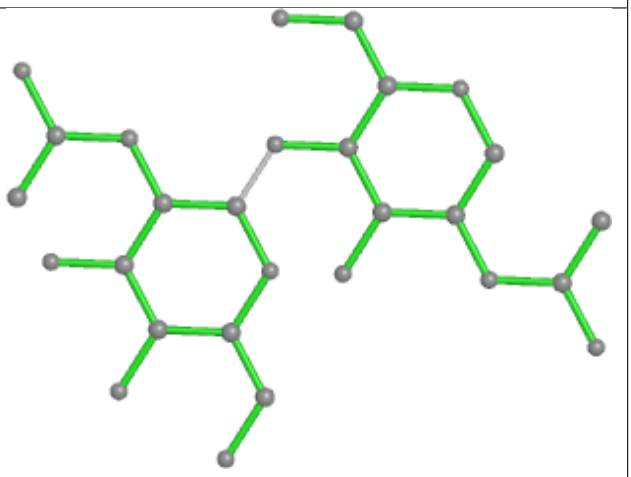


Rings

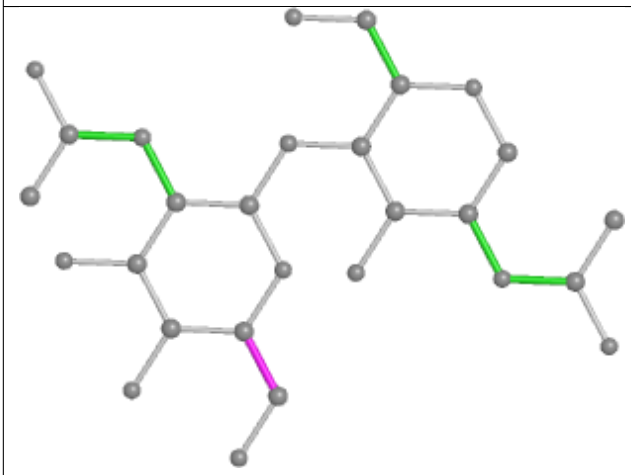
Oligosaccharide Chain M



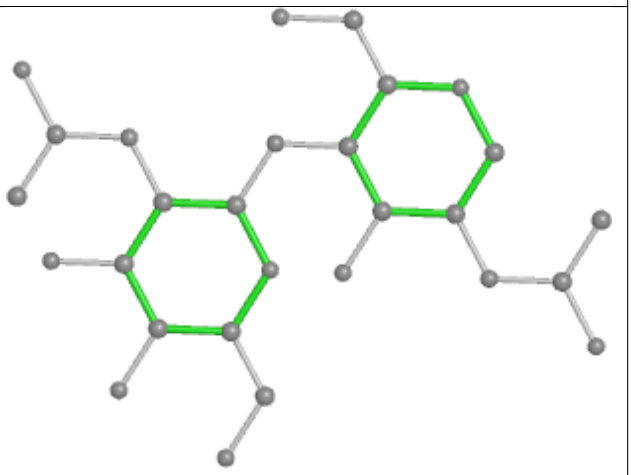
Bond lengths



Bond angles

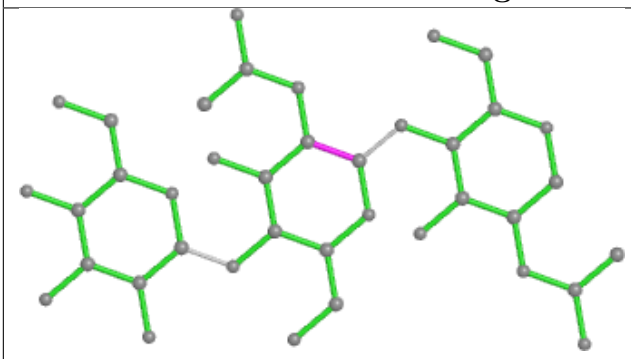


Torsions

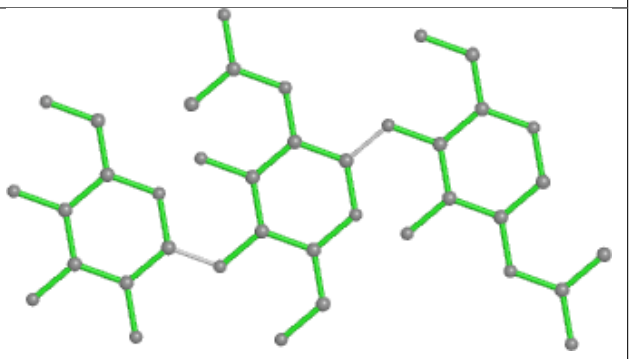


Rings

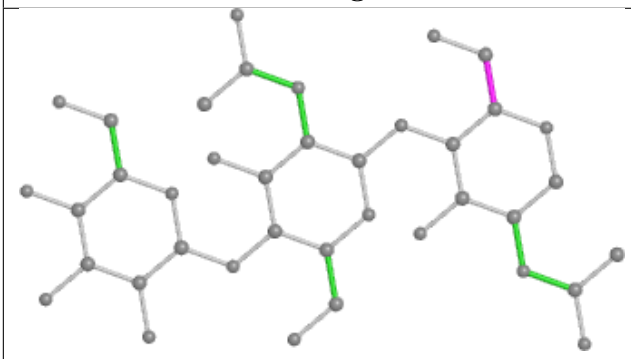
Oligosaccharide Chain K



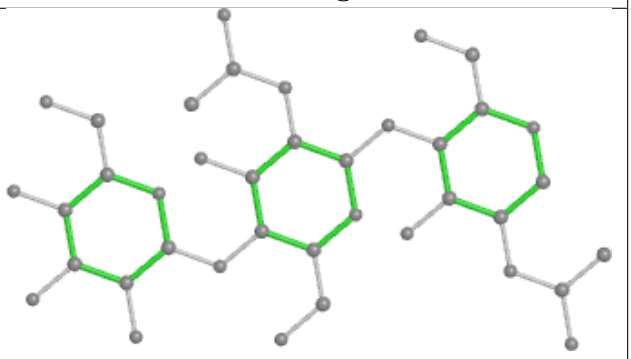
Bond lengths



Bond angles

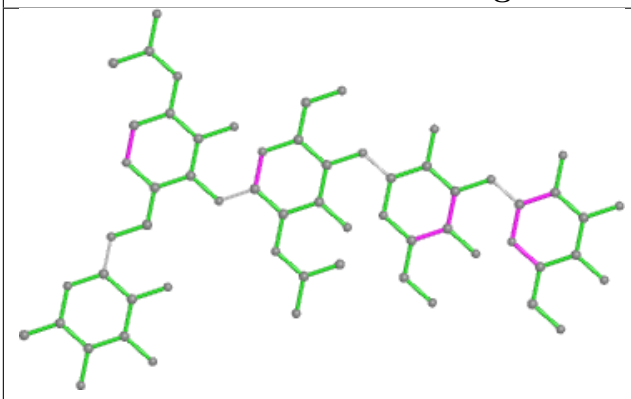


Torsions

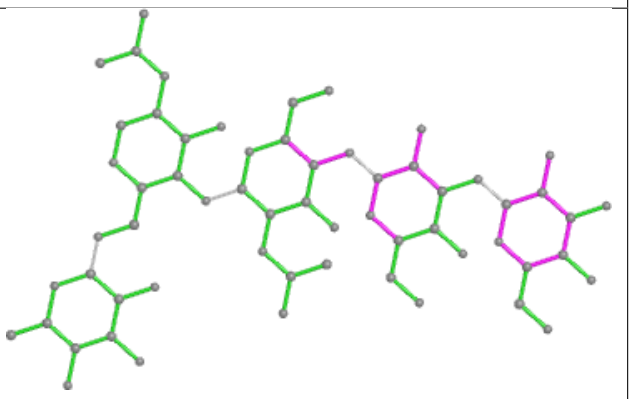


Rings

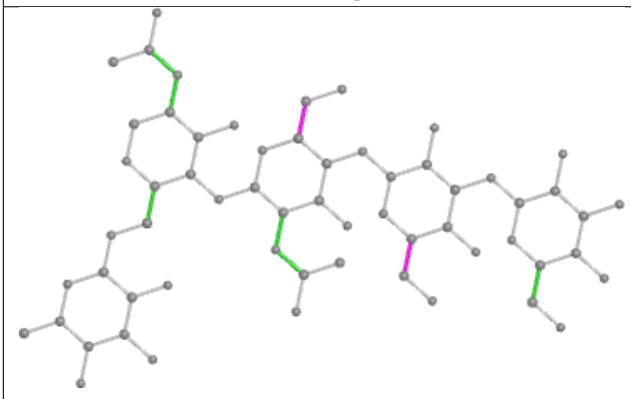
Oligosaccharide Chain N



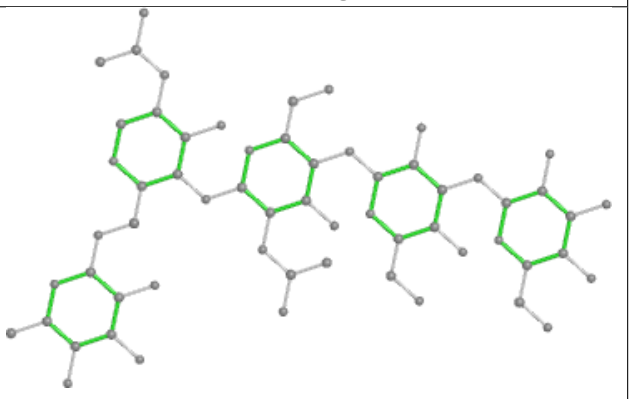
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	H	201	1	14,14,15	0.48	0	17,19,21	0.85	1 (5%)
6	NAG	E	202	1	14,14,15	0.36	0	17,19,21	0.67	0
6	NAG	D	201	-	14,14,15	0.63	1 (7%)	17,19,21	0.38	0
6	NAG	F	201	1	14,14,15	0.20	0	17,19,21	0.55	0
6	NAG	E	201	1	14,14,15	0.65	0	17,19,21	0.71	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	H	201	1	-	0/6/23/26	0/1/1/1
6	NAG	E	202	1	-	0/6/23/26	0/1/1/1
6	NAG	D	201	-	-	0/6/23/26	0/1/1/1
6	NAG	F	201	1	-	2/6/23/26	0/1/1/1
6	NAG	E	201	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	201	NAG	O5-C1	-2.30	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	201	NAG	C1-O5-C5	2.61	115.72	112.19
6	E	201	NAG	C1-O5-C5	2.11	115.05	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

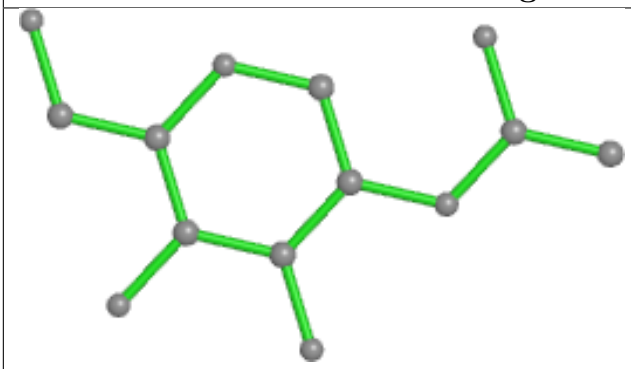
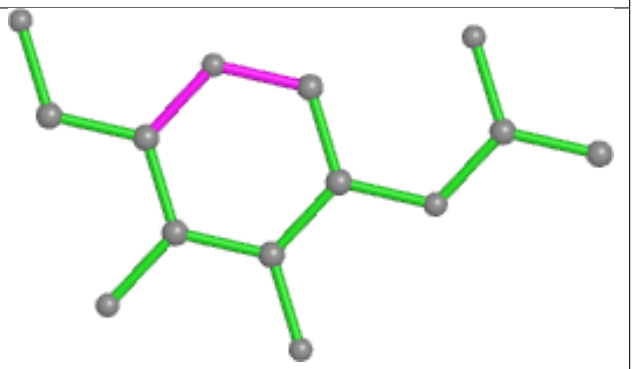
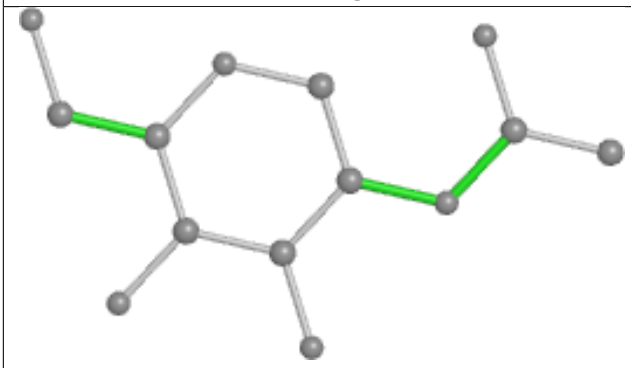
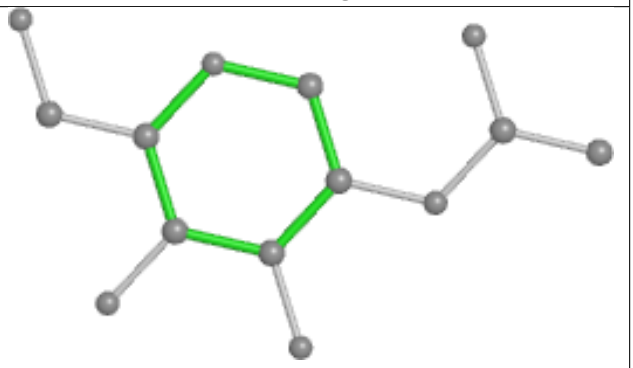
Mol	Chain	Res	Type	Atoms
6	F	201	NAG	O5-C5-C6-O6
6	F	201	NAG	C4-C5-C6-O6

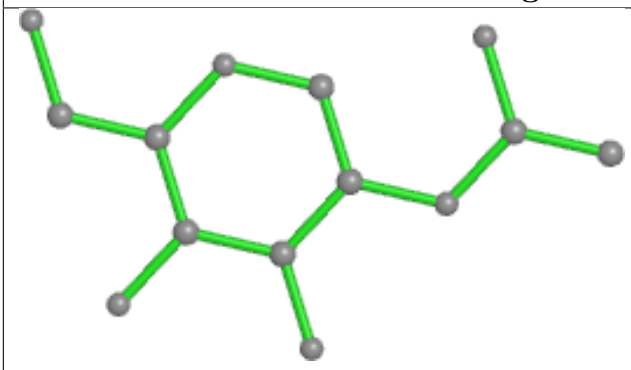
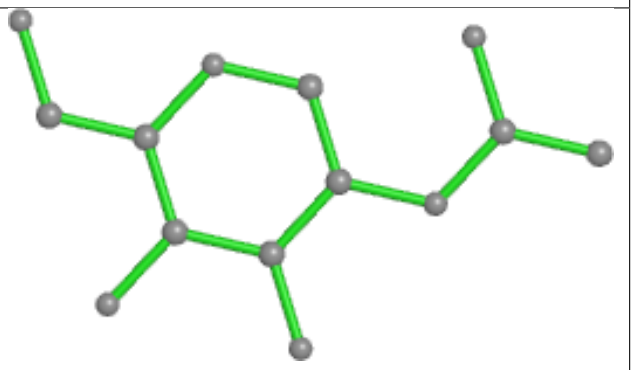
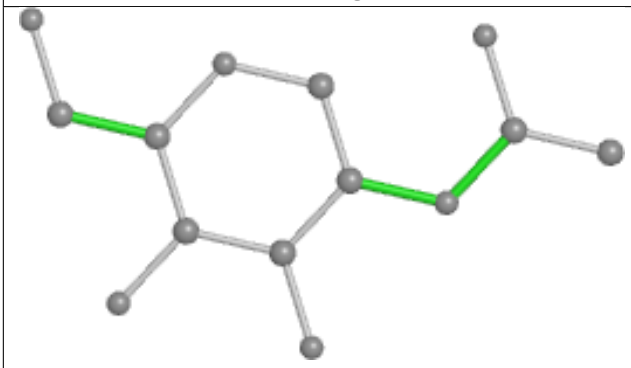
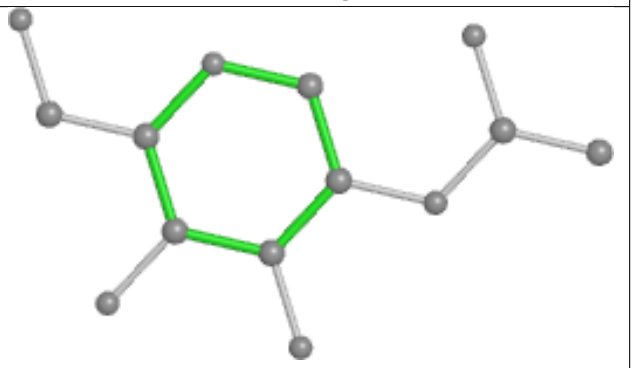
There are no ring outliers.

5 monomers are involved in 7 short contacts:

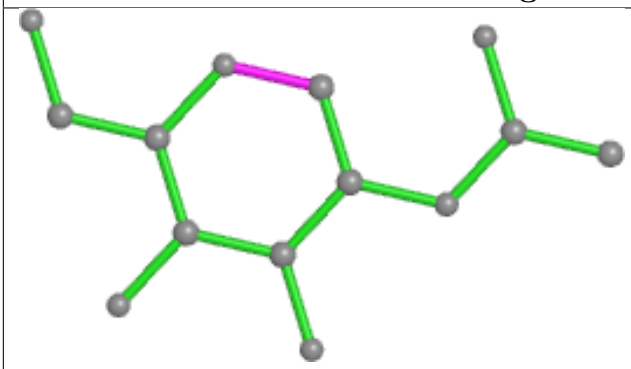
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	201	NAG	1	0
6	E	202	NAG	2	0
6	D	201	NAG	1	0
6	F	201	NAG	1	0
6	E	201	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

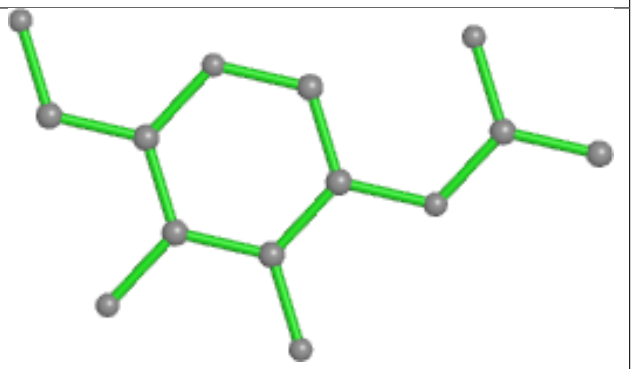
Ligand NAG H 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG E 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

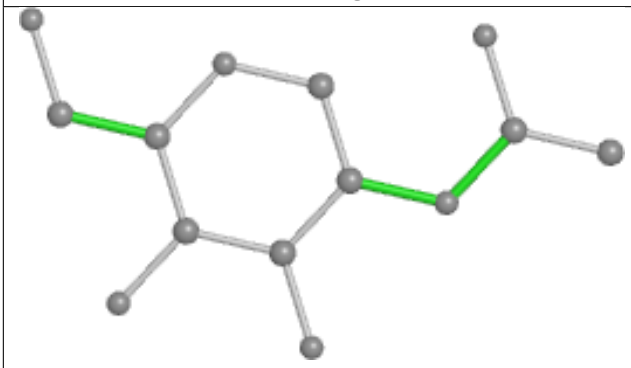
Ligand NAG D 201



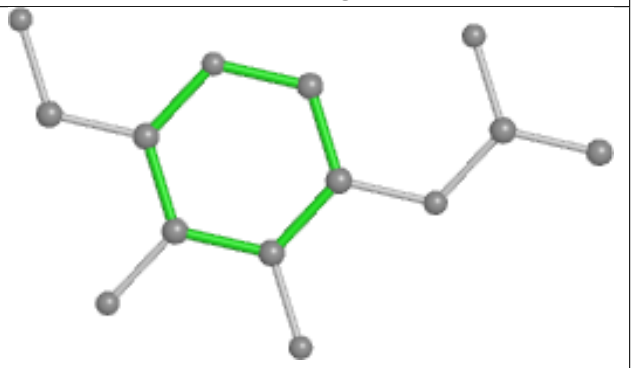
Bond lengths



Bond angles

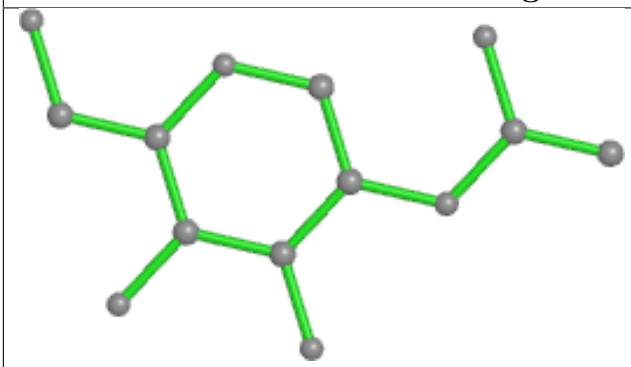


Torsions

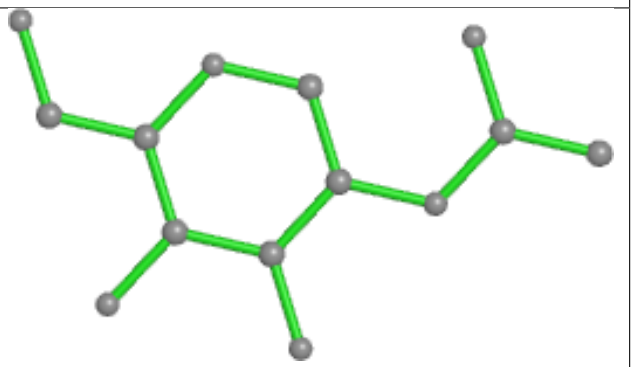


Rings

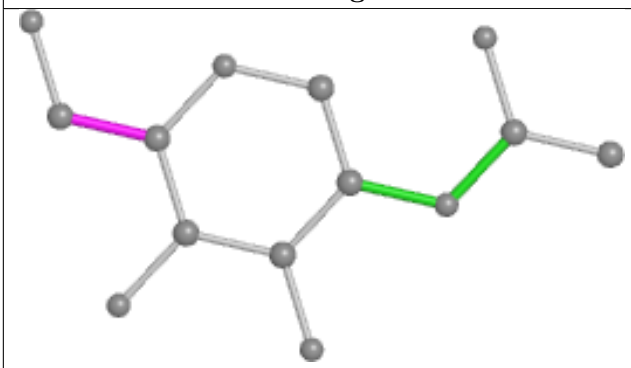
Ligand NAG F 201



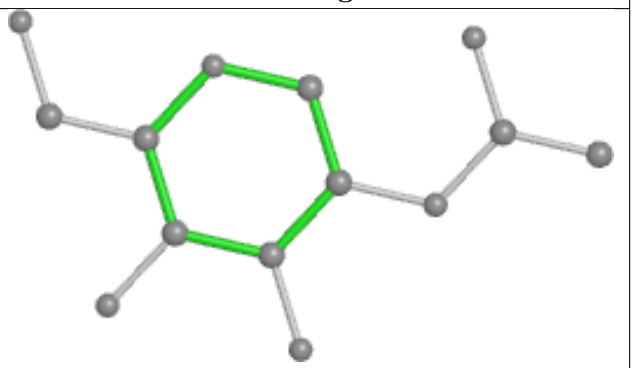
Bond lengths



Bond angles

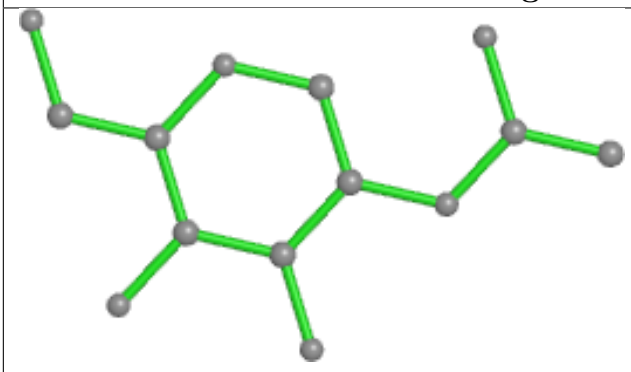


Torsions

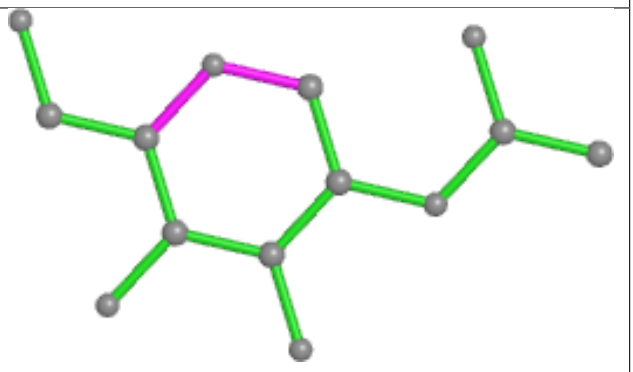


Rings

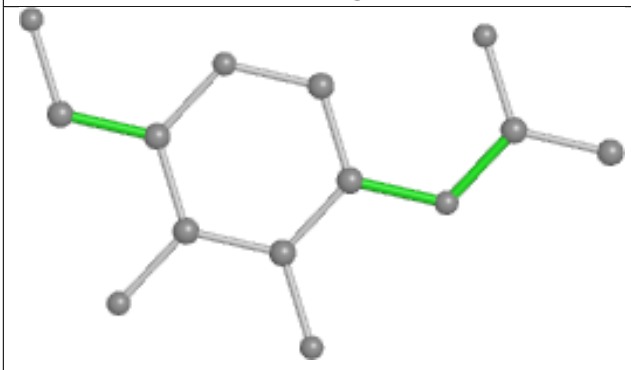
Ligand NAG E 201



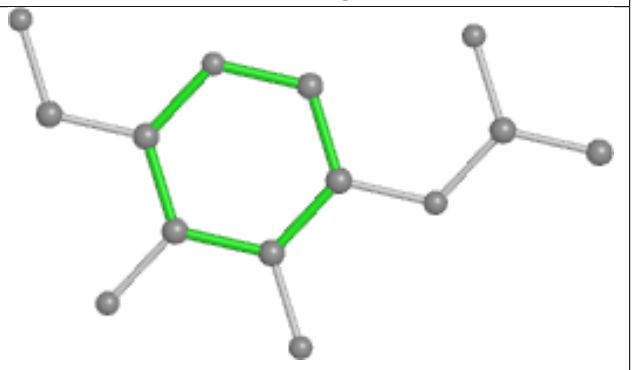
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	129/139 (92%)	0.34	6 (4%)	31	30	17, 34, 93, 134	0
1	B	130/139 (93%)	0.48	7 (5%)	25	24	21, 39, 98, 125	0
1	C	129/139 (92%)	0.39	8 (6%)	20	19	19, 37, 99, 134	0
1	D	128/139 (92%)	0.45	4 (3%)	49	49	19, 38, 82, 116	0
1	E	128/139 (92%)	0.47	5 (3%)	39	38	21, 38, 66, 136	0
1	F	128/139 (92%)	0.54	6 (4%)	31	30	19, 42, 92, 117	0
1	G	128/139 (92%)	0.48	7 (5%)	25	24	25, 43, 85, 103	0
1	H	128/139 (92%)	0.93	20 (15%)	2	1	24, 52, 82, 128	0
All	All	1028/1112 (92%)	0.51	63 (6%)	21	20	17, 40, 92, 136	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	131	THR	6.4
1	B	129	ASN	5.6
1	H	145	ILE	5.3
1	H	113	SER	5.1
1	F	127	HIS	4.8
1	G	128	ASN	4.6
1	E	145	ILE	4.4
1	A	78	PHE	4.3
1	H	78	PHE	4.1
1	G	113	SER	4.1
1	E	75	GLU	4.0
1	D	128	ASN	4.0
1	G	129	ASN	3.9
1	B	130	GLN	3.8
1	B	125	PHE	3.8
1	H	41	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	40	SER	3.6
1	A	76	ASP	3.6
1	H	135	ILE	3.5
1	H	26	PRO	3.5
1	B	127	HIS	3.5
1	G	111	PHE	3.4
1	B	132	VAL	3.3
1	H	37	ILE	3.2
1	H	111	PHE	3.1
1	A	127	HIS	3.1
1	A	125	PHE	3.1
1	C	73	ARG	3.0
1	C	127	HIS	2.9
1	G	127	HIS	2.9
1	A	77	SER	2.9
1	F	125	PHE	2.9
1	F	151	ALA	2.9
1	C	131	THR	2.8
1	H	141	TYR	2.8
1	C	130	GLN	2.7
1	D	76	ASP	2.7
1	H	146	VAL	2.5
1	G	114	ALA	2.5
1	H	125	PHE	2.4
1	F	143	ALA	2.4
1	H	25	ASN	2.3
1	C	36	PHE	2.3
1	E	73	ARG	2.3
1	G	101	THR	2.2
1	E	43	VAL	2.2
1	A	24	SER	2.2
1	H	144	ALA	2.2
1	H	31	VAL	2.2
1	H	76	ASP	2.2
1	E	151	ALA	2.1
1	C	78	PHE	2.1
1	C	77	SER	2.1
1	H	44	ILE	2.1
1	B	78	PHE	2.1
1	F	37	ILE	2.1
1	D	125	PHE	2.1
1	H	130	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	75	GLU	2.0
1	D	75	GLU	2.0
1	H	36	PHE	2.0
1	C	75	GLU	2.0
1	H	148	LEU	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)

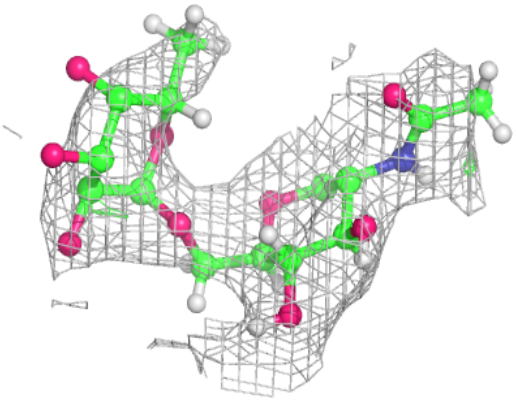
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

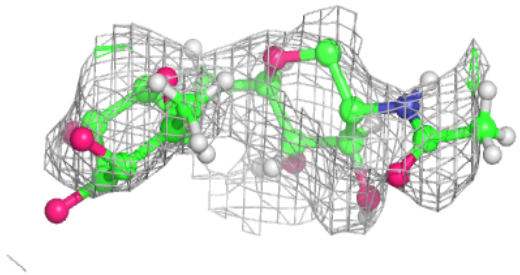
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	L	2	14/15	0.75	0.38	70,97,117,119	0
3	NAG	J	2	14/15	0.76	0.29	67,80,99,119	0
2	FUC	I	2	10/11	0.79	0.26	51,82,99,100	0
4	BMA	K	3	11/12	0.79	0.20	46,63,77,83	0
2	NAG	I	1	14/15	0.81	0.19	64,83,101,107	0
3	NAG	L	1	14/15	0.81	0.21	51,74,98,100	0
3	NAG	M	2	14/15	0.86	0.27	65,81,101,112	0
5	BMA	N	3	11/12	0.86	0.21	50,61,75,84	0
4	NAG	K	2	14/15	0.87	0.22	56,67,72,82	0
4	NAG	K	1	14/15	0.88	0.17	47,63,80,88	0
3	NAG	J	1	14/15	0.88	0.29	53,71,89,99	0
5	NAG	N	2	14/15	0.89	0.18	56,68,78,84	0
5	NAG	N	1	14/15	0.90	0.16	37,55,76,79	0
5	FUC	N	5	10/11	0.90	0.15	58,68,71,81	0
3	NAG	M	1	14/15	0.91	0.18	58,72,88,92	0
5	MAN	N	4	11/12	0.92	0.24	48,58,86,104	0

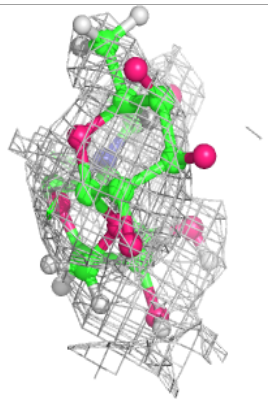
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

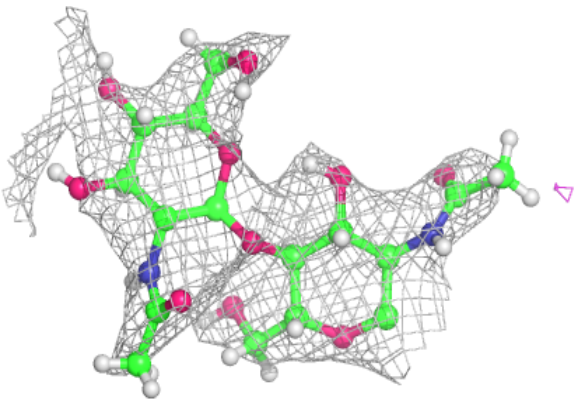


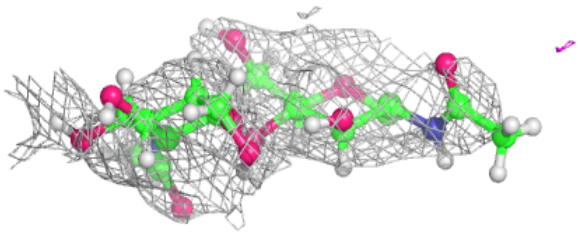


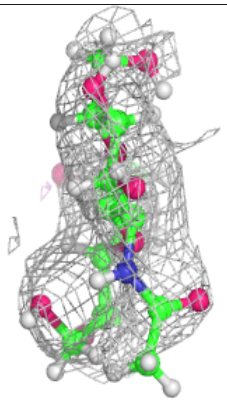


Electron density around Chain J:

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

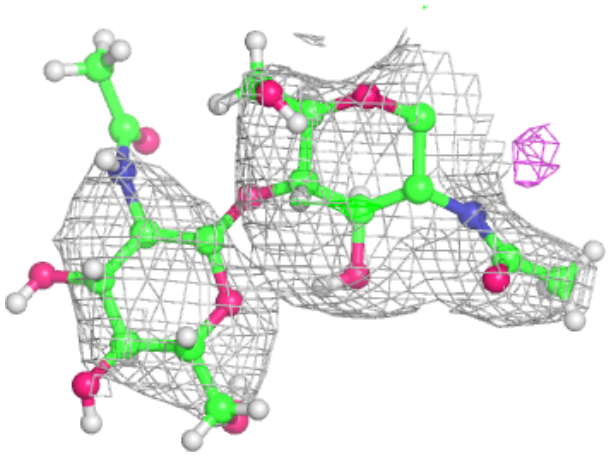


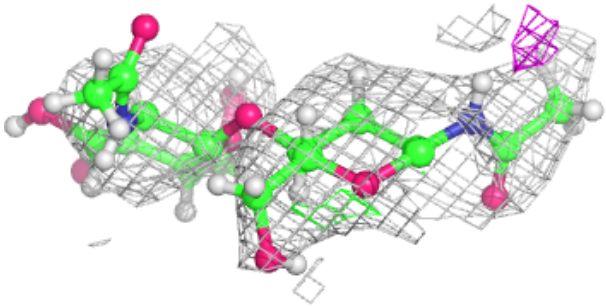


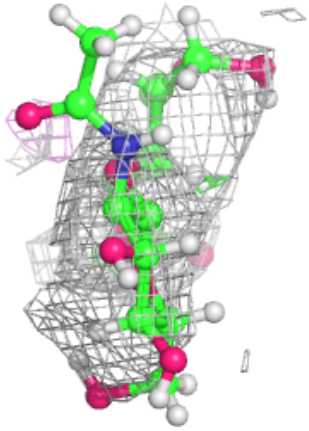


Electron density around Chain L:

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

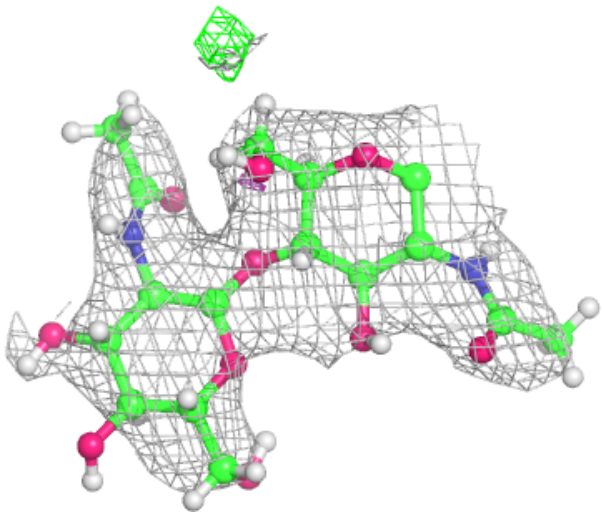


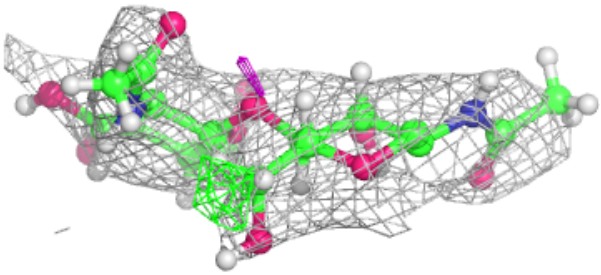


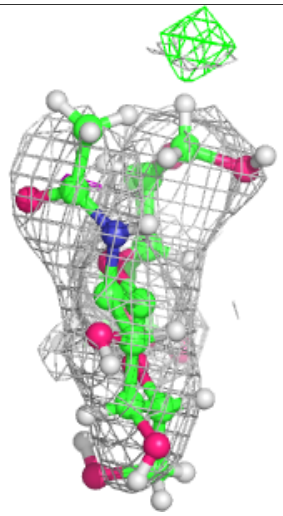


Electron density around Chain M:

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

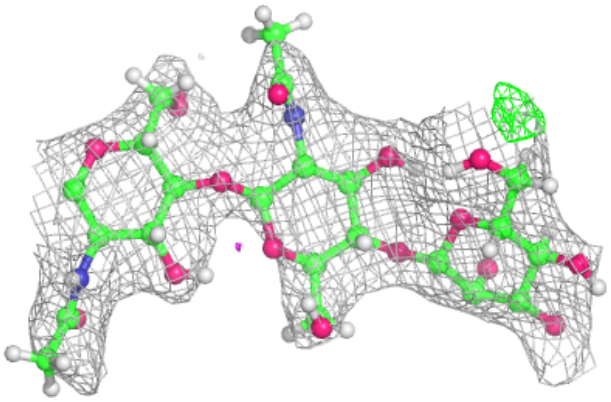


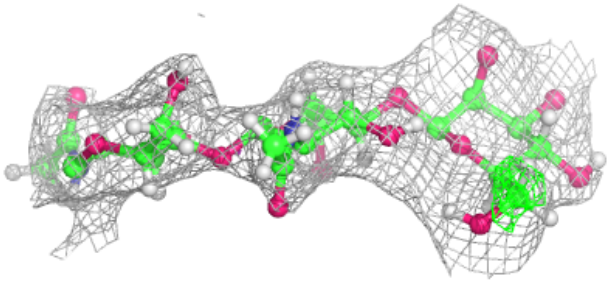


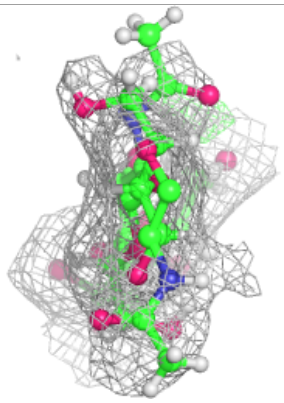


Electron density around Chain K:

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

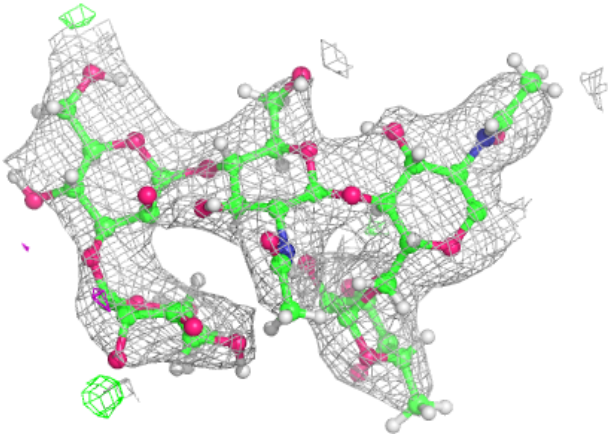


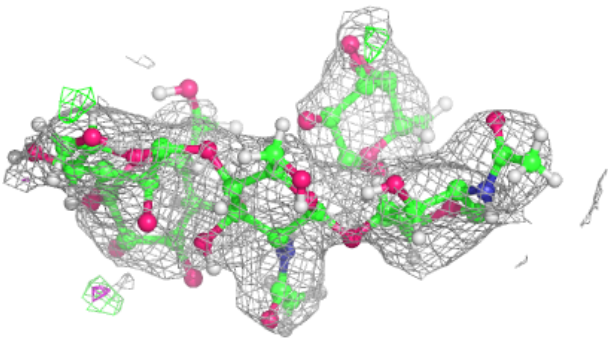


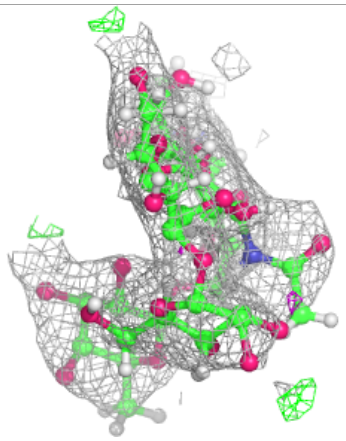


Electron density around Chain N:

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







6.4 Ligands

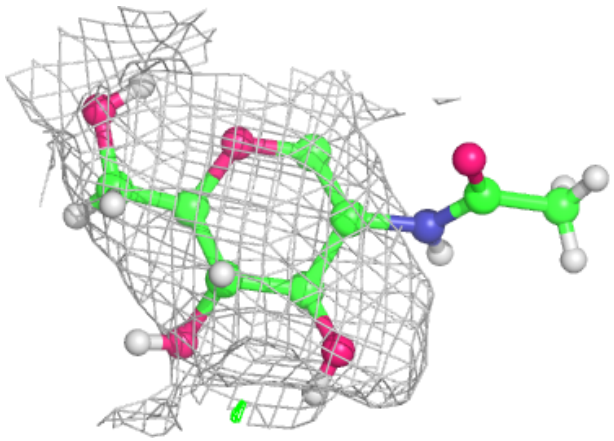
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

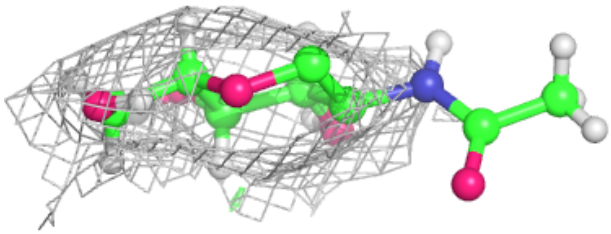
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	F	201	14/15	0.63	0.27	69,84,98,118	0
6	NAG	H	201	14/15	0.71	0.21	76,92,105,111	0
6	NAG	E	201	14/15	0.74	0.23	47,81,102,107	0
6	NAG	D	201	14/15	0.75	0.26	40,66,87,91	0
6	NAG	E	202	14/15	0.85	0.18	36,57,71,73	0

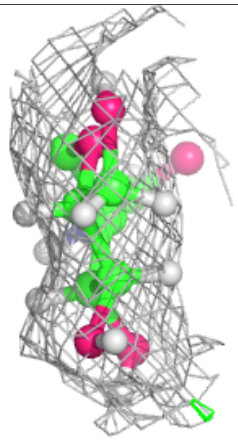
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG F 201:

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

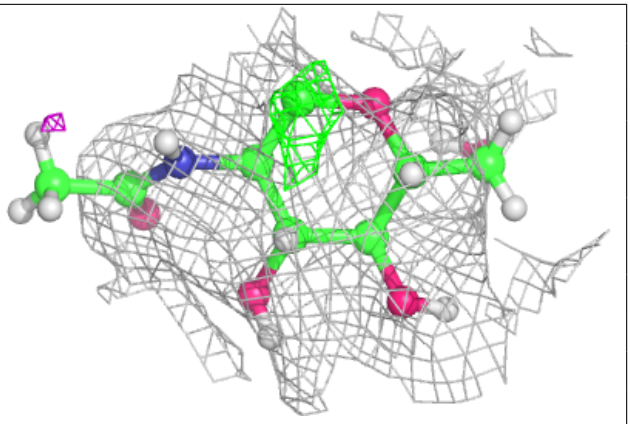


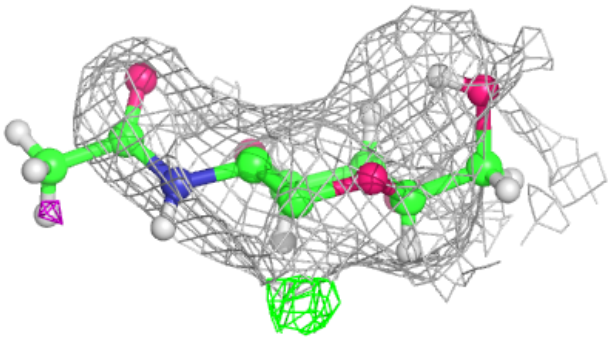


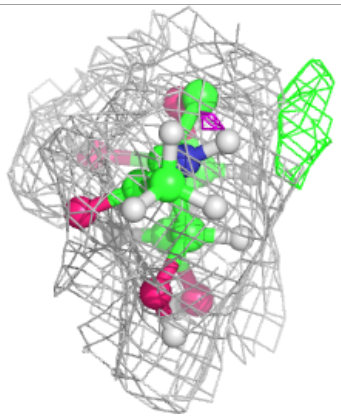


Electron density around NAG H 201:

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

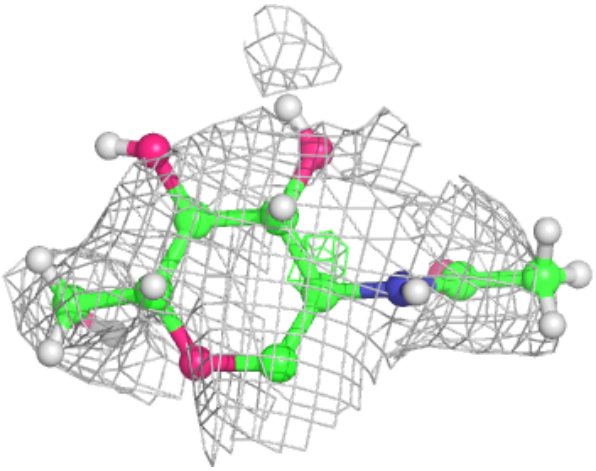


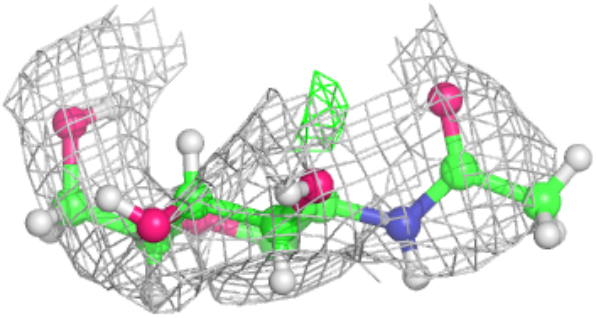


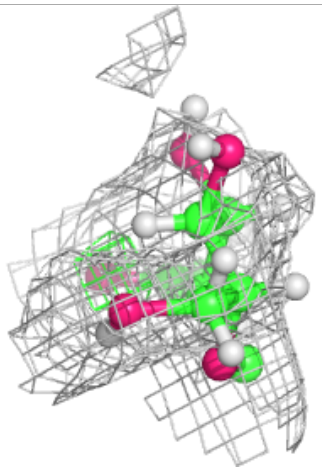


Electron density around NAG E 201:

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

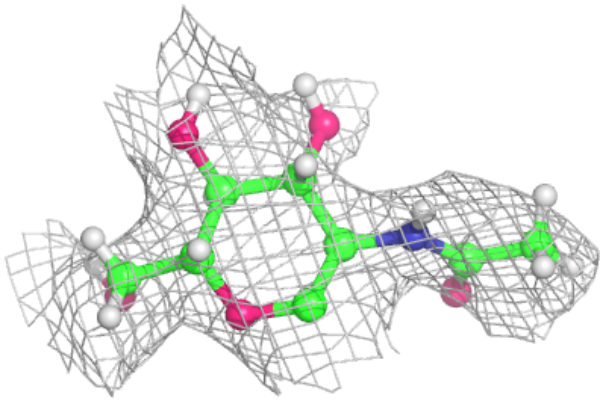


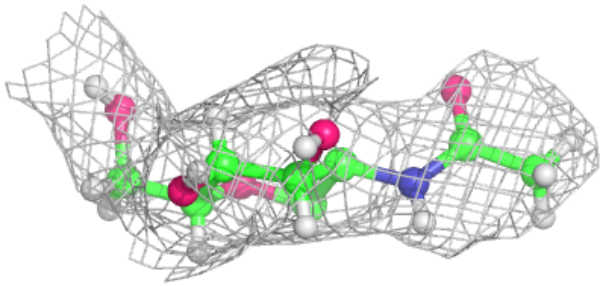


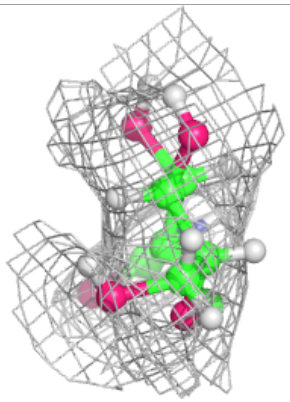


Electron density around NAG D 201:

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

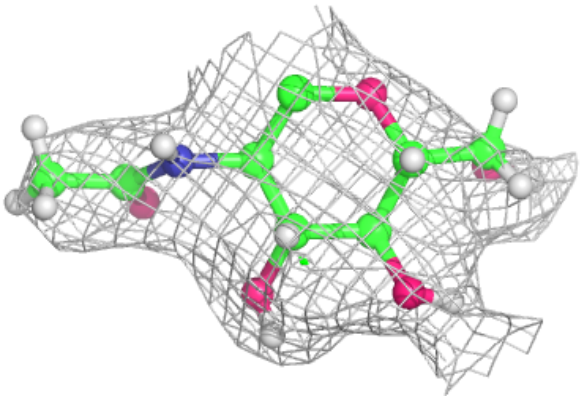


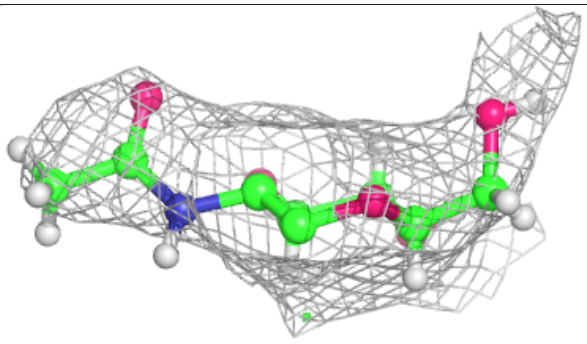


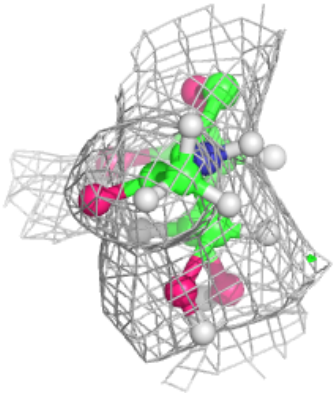


Electron density around NAG E 202:

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







6.5 Other polymers (i)

There are no such residues in this entry.