Full wwPDB X-ray Structure Validation Report (i)

Jan 14, 2024 – 12:20 pm GMT

PDB ID	:	6T3F
Title	:	Crystal structure Nipah virus fusion glycoprotein in complex with a neutralising Fab fragment
Authors	:	Avanzato, V.A.; Pryce, R.; Walter, T.S.; Bowden, T.A.
Deposited on	:	2019-10-10
Resolution	:	3.20 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 (i) 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 (i)) were used in the production of this report:

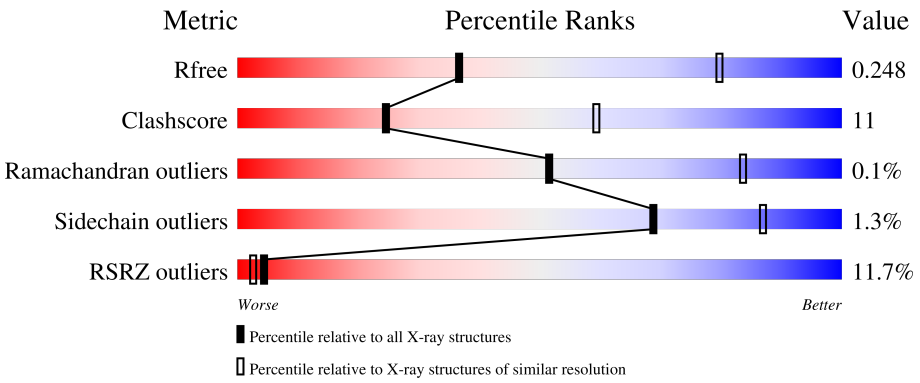
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	F	502	.% 73% 17% 10%
2	L	216	19% 75% 24%
3	H	228	25% 58% 29% • 12%
4	A	2	50% 50%

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	NAG	H	301	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6644 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	F	454	3472	2197	571	684	20	0	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	23	GLU	-	expression tag	UNP Q9IH63
F	24	THR	-	expression tag	UNP Q9IH63
F	25	GLY	-	expression tag	UNP Q9IH63
F	483	GLY	-	expression tag	UNP Q9IH63
F	484	THR	-	expression tag	UNP Q9IH63
F	485	MET	-	expression tag	UNP Q9IH63
F	486	LYS	-	expression tag	UNP Q9IH63
F	487	GLN	-	expression tag	UNP Q9IH63
F	488	ILE	-	expression tag	UNP Q9IH63
F	489	GLU	-	expression tag	UNP Q9IH63
F	490	ASP	-	expression tag	UNP Q9IH63
F	491	LYS	-	expression tag	UNP Q9IH63
F	492	ILE	-	expression tag	UNP Q9IH63
F	493	GLU	-	expression tag	UNP Q9IH63
F	494	GLU	-	expression tag	UNP Q9IH63
F	495	ILE	-	expression tag	UNP Q9IH63
F	496	LEU	-	expression tag	UNP Q9IH63
F	497	SER	-	expression tag	UNP Q9IH63
F	498	LYS	-	expression tag	UNP Q9IH63
F	499	ILE	-	expression tag	UNP Q9IH63
F	500	TYR	-	expression tag	UNP Q9IH63
F	501	HIS	-	expression tag	UNP Q9IH63
F	502	ILE	-	expression tag	UNP Q9IH63
F	503	GLU	-	expression tag	UNP Q9IH63
F	504	ASN	-	expression tag	UNP Q9IH63
F	505	GLU	-	expression tag	UNP Q9IH63
F	506	ILE	-	expression tag	UNP Q9IH63

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Chain	Residue	Modelled	Actual	Comment	Reference
F	507	ALA	-	expression tag	UNP Q9IH63
F	508	ARG	-	expression tag	UNP Q9IH63
F	509	ILE	-	expression tag	UNP Q9IH63
F	510	LYS	-	expression tag	UNP Q9IH63
F	511	LYS	-	expression tag	UNP Q9IH63
F	512	LEU	-	expression tag	UNP Q9IH63
F	513	ILE	-	expression tag	UNP Q9IH63
F	514	GLY	-	expression tag	UNP Q9IH63
F	515	GLU	-	expression tag	UNP Q9IH63
F	516	GLY	-	expression tag	UNP Q9IH63
F	517	GLY	-	expression tag	UNP Q9IH63
F	518	SER	-	expression tag	UNP Q9IH63
F	519	HIS	-	expression tag	UNP Q9IH63
F	520	HIS	-	expression tag	UNP Q9IH63
F	521	HIS	-	expression tag	UNP Q9IH63
F	522	HIS	-	expression tag	UNP Q9IH63
F	523	HIS	-	expression tag	UNP Q9IH63
F	524	HIS	-	expression tag	UNP Q9IH63

- Molecule 2 is a protein called Fab66 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	215	1602	1005	260	329	8	0	0	0

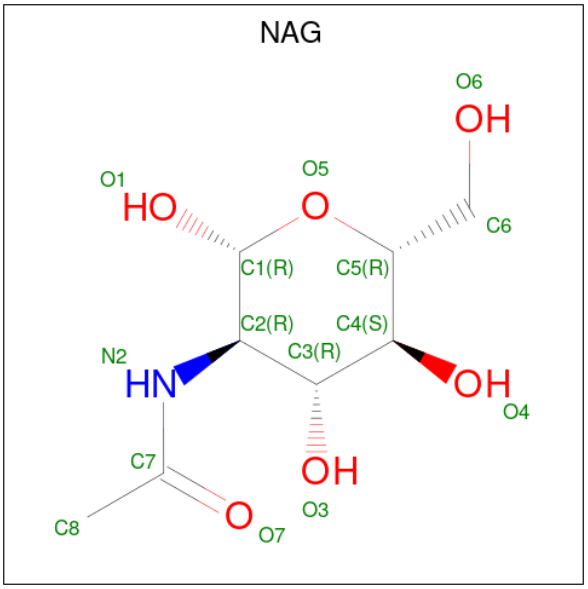
- Molecule 3 is a protein called Fab66 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	201	1486	941	251	284	10	0	0	0

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

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

- Molecule 5 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).

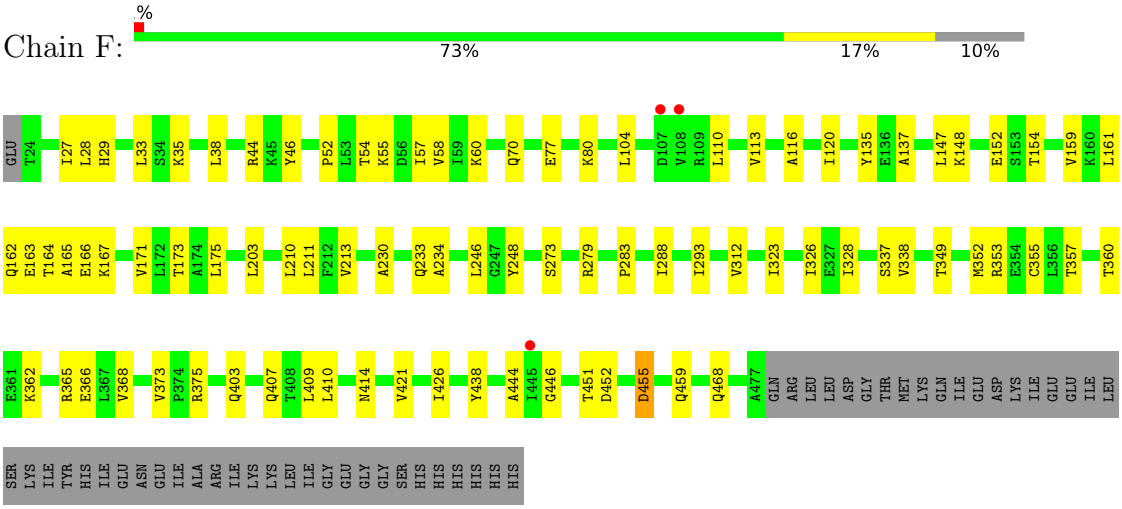


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	F	1	14	8	1	5	0	0
			Total	C	N	O		
5	F	1	14	8	1	5	0	0
			Total	C	N	O		
5	F	1	14	8	1	5	0	0
			Total	C	N	O		
5	H	1	14	8	1	5	0	0

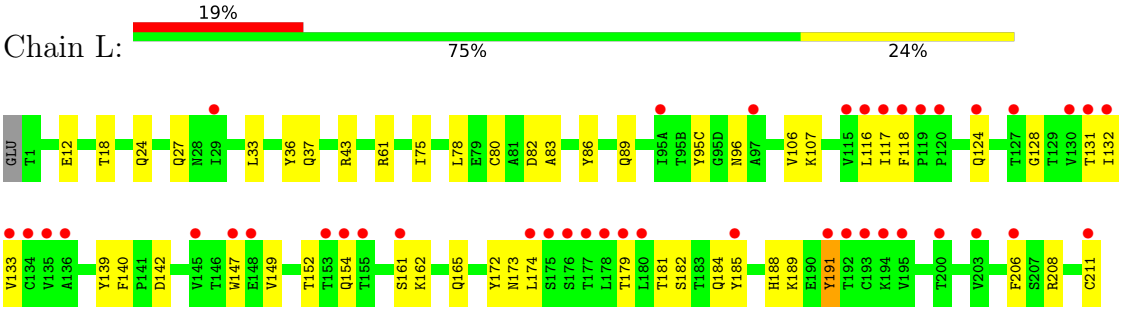
3 Residue-property plots (i)

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.

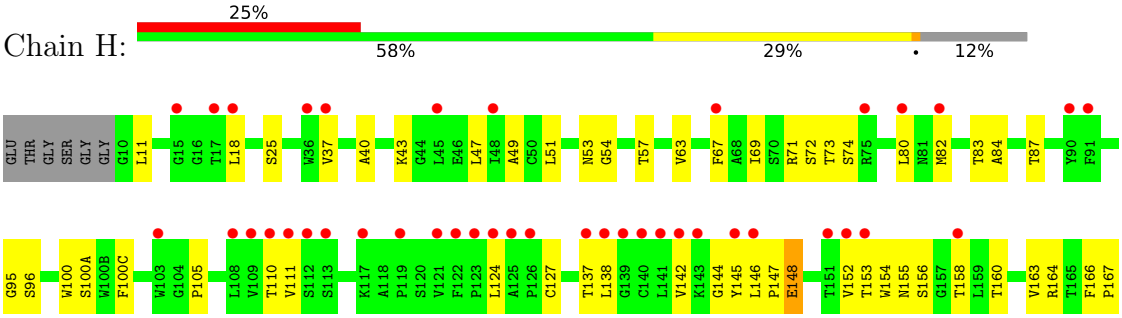
• Molecule 1: Fusion glycoprotein F0

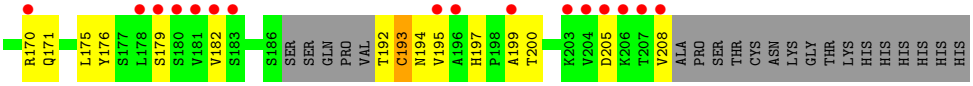


• Molecule 2: Fab66 light chain



• Molecule 3: Fab66 heavy chain





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

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	149.25Å 149.25Å 385.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	91.12 – 3.20 91.12 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (91.12-3.20) 99.5 (91.12-3.20)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 3.19Å)	Xtriage
Refinement program	PHENIX dev_3488	Depositor
R, R_{free}	0.213 , 0.248 0.213 , 0.248	Depositor DCC
R_{free} test set	2114 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	93.8	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 91.3	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	0.93	EDS
Total number of atoms	6644	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	F	0.26	0/3521	0.46	0/4785
2	L	0.26	0/1635	0.48	0/2237
3	H	0.26	0/1525	0.51	0/2091
All	All	0.26	0/6681	0.48	0/9113

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3472	0	3517	54	0
2	L	1602	0	1557	43	0
3	H	1486	0	1457	59	0
4	A	28	0	25	1	0
5	F	42	0	39	1	0
5	H	14	0	13	0	0
All	All	6644	0	6608	144	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 11.

All (144) 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)
3:H:155:ASN:HD21	3:H:158:THR:HG22	1.38	0.86
3:H:49:ALA:HB1	3:H:69:ILE:HD11	1.59	0.84
3:H:144:GLY:HA2	3:H:175:LEU:HD12	1.62	0.81
3:H:155:ASN:HB3	3:H:192:THR:HA	1.69	0.75
1:F:365:ARG:NH2	1:F:446:GLY:O	2.21	0.74
2:L:211:CYS:N	3:H:127:CYS:SG	2.60	0.74
2:L:96:ASN:HB2	3:H:100:TRP:HZ3	1.52	0.73
1:F:452:ASP:HB3	1:F:455:ASP:HB2	1.70	0.72
3:H:63:VAL:HG23	3:H:67:PHE:HD2	1.57	0.70
3:H:95:GLY:O	3:H:100(A):SER:OG	2.09	0.69
2:L:124:GLN:NE2	2:L:131:THR:O	2.23	0.69
3:H:153:THR:OG1	3:H:194:ASN:OD1	2.10	0.68
1:F:163:GLU:HG2	1:F:164:THR:HG22	1.76	0.67
3:H:54:GLY:HA3	3:H:71:ARG:HH22	1.59	0.66
1:F:80:LYS:NZ	2:L:95(C):TYR:OH	2.29	0.66
1:F:57:ILE:HB	1:F:246:LEU:HD21	1.77	0.66
3:H:156:SER:H	3:H:194:ASN:HD21	1.43	0.65
2:L:149:VAL:HG12	2:L:154:GLN:NE2	2.12	0.64
1:F:38:LEU:HD11	1:F:312:VAL:HG21	1.79	0.63
3:H:154:TRP:HD1	3:H:193:CYS:HA	1.63	0.63
1:F:163:GLU:N	1:F:163:GLU:OE1	2.33	0.62
2:L:139:TYR:HE1	2:L:174:LEU:HD23	1.63	0.62
2:L:83:ALA:HB2	2:L:106:VAL:HG22	1.81	0.61
1:F:152:GLU:OE1	1:F:273:SER:OG	2.18	0.61
2:L:89:GLN:HE22	3:H:100(C):PHE:HE2	1.47	0.60
1:F:360:THR:OG1	1:F:444:ALA:O	2.20	0.60
2:L:116:LEU:HD21	3:H:137:THR:HG21	1.82	0.60
3:H:148:GLU:HG2	3:H:176:TYR:CZ	2.38	0.58
2:L:61:ARG:NH2	2:L:82:ASP:OD2	2.36	0.58
2:L:149:VAL:HG12	2:L:154:GLN:HE21	1.69	0.57
1:F:54:THR:HB	1:F:279:ARG:HH21	1.68	0.57
2:L:43:ARG:HD3	3:H:105:PRO:HA	1.86	0.57
1:F:29:HIS:ND1	1:F:357:THR:O	2.37	0.57
3:H:53:ASN:OD1	3:H:54:GLY:N	2.37	0.57
2:L:152:THR:O	2:L:154:GLN:NE2	2.38	0.57
2:L:184:GLN:O	2:L:188:HIS:ND1	2.33	0.57
2:L:149:VAL:H	2:L:154:GLN:HE22	1.51	0.56
2:L:96:ASN:HB2	3:H:100:TRP:CZ3	2.38	0.55
2:L:139:TYR:CE1	2:L:174:LEU:HD23	2.41	0.55
1:F:159:VAL:HG12	1:F:171:VAL:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:67:PHE:HB3	3:H:80:LEU:HD11	1.89	0.55
1:F:366:GLU:OE1	1:F:451:THR:OG1	2.18	0.55
3:H:51:LEU:HD23	3:H:57:THR:HG22	1.87	0.55
1:F:27:ILE:HG13	1:F:28:LEU:HD12	1.88	0.55
2:L:165:GLN:HG2	2:L:172:TYR:CE1	2.42	0.54
2:L:189:LYS:O	2:L:208:ARG:HB2	2.08	0.54
3:H:138:LEU:O	3:H:182:VAL:N	2.36	0.54
3:H:87:THR:HG23	3:H:111:VAL:HG22	1.88	0.54
3:H:192:THR:HG23	3:H:208:VAL:HG13	1.90	0.53
2:L:33:LEU:HD12	2:L:89:GLN:O	2.07	0.53
3:H:194:ASN:HB3	3:H:205:ASP:HB3	1.91	0.53
2:L:185:TYR:O	2:L:191:TYR:OH	2.28	0.52
2:L:36:TYR:HE2	2:L:89:GLN:HG2	1.74	0.52
1:F:455:ASP:O	1:F:459:GLN:HG3	2.09	0.52
1:F:164:THR:HG23	1:F:166:GLU:HB3	1.91	0.52
3:H:154:TRP:HE3	3:H:163:VAL:HG22	1.74	0.51
1:F:104:LEU:HB2	1:F:110:LEU:HD11	1.92	0.51
3:H:154:TRP:CD1	3:H:193:CYS:HA	2.43	0.51
1:F:414:ASN:ND2	5:F:605:NAG:H83	2.25	0.51
3:H:152:VAL:HG22	3:H:195:VAL:HG22	1.92	0.51
3:H:95:GLY:HA2	3:H:100(C):PHE:HA	1.93	0.51
2:L:211:CYS:SG	3:H:127:CYS:N	2.84	0.51
3:H:154:TRP:CE3	3:H:163:VAL:HG22	2.46	0.51
2:L:37:GLN:HB2	2:L:86:TYR:HE1	1.77	0.50
1:F:213:VAL:HG21	1:F:233:GLN:HG3	1.94	0.50
3:H:54:GLY:CA	3:H:71:ARG:HH22	2.24	0.49
2:L:78:LEU:HD13	2:L:106:VAL:HG12	1.94	0.49
3:H:154:TRP:CZ3	3:H:182:VAL:HB	2.47	0.49
3:H:37:VAL:HG22	3:H:47:LEU:HD21	1.95	0.49
3:H:170:ARG:HG2	3:H:176:TYR:CE1	2.48	0.49
1:F:175:LEU:HD12	1:F:203:LEU:HD23	1.96	0.48
3:H:197:HIS:CE1	3:H:200:THR:HG1	2.30	0.48
1:F:293:ILE:HD12	1:F:338:VAL:HB	1.95	0.48
1:F:368:VAL:HG11	1:F:373:VAL:HG11	1.95	0.48
1:F:70:GLN:HB3	3:H:100(A):SER:HB3	1.96	0.48
3:H:146:LEU:HB3	3:H:147:PRO:HD3	1.95	0.47
1:F:162:GLN:HE21	1:F:165:ALA:HA	1.80	0.47
2:L:173:ASN:ND2	3:H:164:ARG:HD3	2.30	0.47
2:L:181:THR:HG22	2:L:184:GLN:OE1	2.15	0.47
3:H:83:THR:OG1	3:H:84:ALA:N	2.47	0.47
2:L:12:GLU:HB3	2:L:107:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:124:GLN:NE2	2:L:131:THR:H	2.13	0.47
1:F:403:GLN:HG3	1:F:407:GLN:HG3	1.97	0.47
2:L:61:ARG:HH22	2:L:82:ASP:CG	2.19	0.47
2:L:161:SER:HB2	3:H:167:PRO:HG2	1.96	0.47
3:H:155:ASN:O	3:H:155:ASN:ND2	2.48	0.47
3:H:160:THR:HA	3:H:163:VAL:HG23	1.96	0.46
2:L:162:LYS:HD2	2:L:172:TYR:CD1	2.51	0.46
3:H:145:TYR:CZ	3:H:176:TYR:HB2	2.49	0.46
1:F:113:VAL:HG11	1:F:135:TYR:CZ	2.50	0.46
3:H:84:ALA:O	3:H:87:THR:OG1	2.31	0.46
3:H:142:VAL:HG21	3:H:195:VAL:HG11	1.98	0.46
1:F:137:ALA:HA	1:F:279:ARG:NH1	2.31	0.46
3:H:47:LEU:HA	3:H:47:LEU:HD23	1.66	0.46
3:H:194:ASN:HA	3:H:205:ASP:HB3	1.97	0.46
1:F:58:VAL:HB	1:F:171:VAL:HG22	1.97	0.45
3:H:40:ALA:HB3	3:H:43:LYS:HB2	1.98	0.45
1:F:60:LYS:HB3	1:F:173:THR:HG23	1.99	0.45
1:F:210:LEU:HD12	1:F:234:ALA:HA	1.98	0.45
3:H:145:TYR:CE1	3:H:176:TYR:HB2	2.52	0.45
3:H:87:THR:HG22	3:H:110:THR:HA	1.99	0.44
1:F:326:ILE:HG23	1:F:328:ILE:HG12	1.99	0.44
1:F:355:CYS:HB2	1:F:362:LYS:HB2	2.00	0.44
3:H:197:HIS:CE1	3:H:199:ALA:HB3	2.53	0.44
1:F:77:GLU:OE2	2:L:95(C):TYR:OH	2.35	0.44
1:F:323:ILE:O	1:F:353:ARG:NH2	2.50	0.44
1:F:44:ARG:HB3	1:F:337:SER:HA	1.99	0.44
1:F:33:LEU:HD22	1:F:38:LEU:HD12	2.00	0.44
3:H:72:SER:C	3:H:74:SER:H	2.20	0.43
1:F:421:VAL:HG22	1:F:426:ILE:HG12	1.99	0.43
3:H:67:PHE:CE1	3:H:82:MET:HG2	2.52	0.43
3:H:138:LEU:HD23	3:H:138:LEU:HA	1.77	0.43
1:F:373:VAL:O	1:F:375:ARG:HG3	2.19	0.43
1:F:211:LEU:HD23	1:F:211:LEU:HA	1.81	0.43
3:H:72:SER:O	3:H:74:SER:N	2.51	0.43
3:H:11:LEU:HD12	3:H:11:LEU:O	2.19	0.42
1:F:148:LYS:O	1:F:152:GLU:HG3	2.19	0.42
1:F:409:LEU:HD23	1:F:409:LEU:HA	1.86	0.42
1:F:147:LEU:HD23	1:F:161:LEU:HD23	2.01	0.42
1:F:52:PRO:HA	1:F:283:PRO:HA	2.00	0.42
2:L:124:GLN:HE21	2:L:131:THR:H	1.67	0.42
2:L:128:GLY:HA2	2:L:182:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:VAL:HG11	1:F:230:ALA:O	2.20	0.42
2:L:117:ILE:HD13	2:L:206:PHE:CD1	2.54	0.42
1:F:410:LEU:HD23	1:F:410:LEU:HA	1.81	0.42
1:F:35:LYS:HG2	1:F:438:TYR:CZ	2.55	0.41
1:F:349:THR:HG23	1:F:352:MET:H	1.85	0.41
1:F:46:TYR:HB3	1:F:288:ILE:HB	2.02	0.41
2:L:107:LYS:HA	2:L:140:PHE:CZ	2.55	0.41
3:H:155:ASN:O	3:H:156:SER:OG	2.32	0.41
1:F:167:LYS:HD3	1:F:167:LYS:HA	1.86	0.41
1:F:55:LYS:HD2	1:F:248:TYR:CZ	2.56	0.41
2:L:131:THR:HG23	2:L:179:THR:HG23	2.02	0.41
1:F:468:GLN:HG2	4:A:1:NAG:H61	2.03	0.41
1:F:116:ALA:O	1:F:120:ILE:HG12	2.21	0.41
2:L:18:THR:HA	2:L:75:ILE:O	2.21	0.41
2:L:118:PHE:HB2	2:L:133:VAL:HG22	2.02	0.41
2:L:132:ILE:HG22	2:L:147:TRP:HH2	1.86	0.41
3:H:25:SER:O	3:H:25:SER:OG	2.28	0.40
3:H:166:PHE:HB2	3:H:179:SER:O	2.20	0.40
1:F:60:LYS:HE2	1:F:154:THR:OG1	2.22	0.40
1:F:55:LYS:HD2	1:F:248:TYR:CE1	2.56	0.40
2:L:80:CYS:HA	2:L:106:VAL:HG21	2.03	0.40
2:L:142:ASP:OD1	2:L:162:LYS:NZ	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	452/502 (90%)	437 (97%)	15 (3%)	0	100	100
2	L	213/216 (99%)	199 (93%)	14 (7%)	0	100	100
3	H	197/228 (86%)	185 (94%)	11 (6%)	1 (0%)	29	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	862/946 (91%)	821 (95%)	40 (5%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	73	THR

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	F	398/444 (90%)	397 (100%)	1 (0%)	92 96
2	L	180/181 (99%)	177 (98%)	3 (2%)	60 83
3	H	167/189 (88%)	161 (96%)	6 (4%)	35 69
All	All	745/814 (92%)	735 (99%)	10 (1%)	69 87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	455	ASP
2	L	24	GLN
2	L	27	GLN
2	L	191	TYR
3	H	18	LEU
3	H	96	SER
3	H	124	LEU
3	H	148	GLU
3	H	171	GLN
3	H	193	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	89	GLN
2	L	124	GLN
2	L	154	GLN
3	H	155	ASN

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)

2 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	$\#\|Z\| > 2$
4	NAG	A	1	1,4	14,14,15	0.67	1 (7%)	17,19,21	0.63	0
4	NAG	A	2	4	14,14,15	0.57	0	17,19,21	1.02	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
4	NAG	A	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	A	2	4	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	NAG	O5-C1	2.10	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2	NAG	C1-C2-N2	2.73	115.14	110.49
4	A	2	NAG	C2-N2-C7	2.53	126.51	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2	NAG	O5-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6
4	A	1	NAG	O5-C5-C6-O6
4	A	2	NAG	C3-C2-N2-C7
4	A	1	NAG	C4-C5-C6-O6

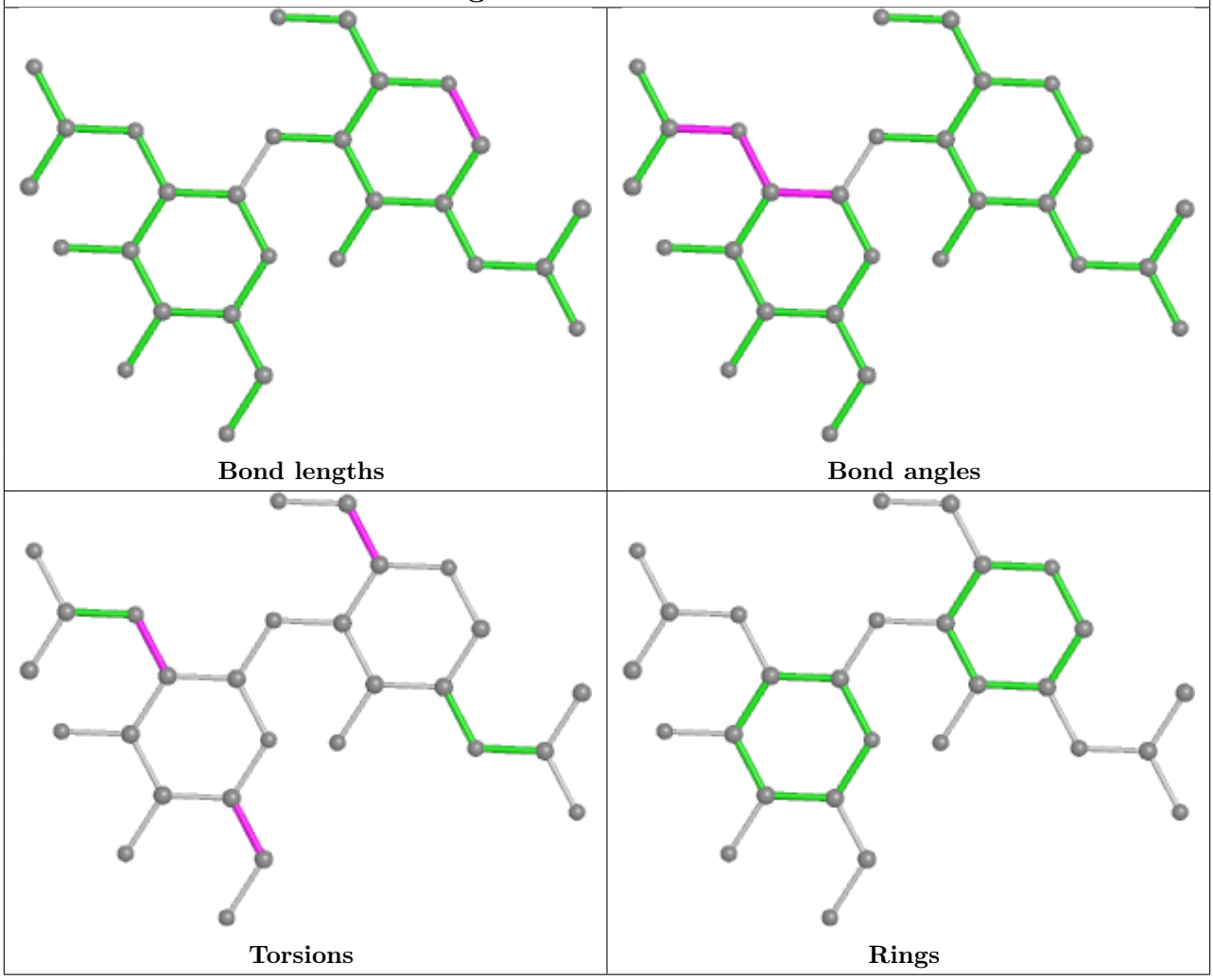
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	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 A



5.6 Ligand geometry (i)

4 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	F	605	1	14,14,15	0.45	0	17,19,21	0.64	1 (5%)
5	NAG	F	602	1	14,14,15	0.27	0	17,19,21	0.58	0
5	NAG	F	601	1	14,14,15	0.24	0	17,19,21	0.48	0
5	NAG	H	301	3	14,14,15	0.20	0	17,19,21	0.47	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
5	NAG	F	605	1	-	4/6/23/26	0/1/1/1
5	NAG	F	602	1	-	2/6/23/26	0/1/1/1
5	NAG	F	601	1	-	2/6/23/26	0/1/1/1
5	NAG	H	301	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	605	NAG	C1-O5-C5	2.02	114.92	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	605	NAG	C8-C7-N2-C2
5	F	605	NAG	O7-C7-N2-C2
5	H	301	NAG	O5-C5-C6-O6
5	H	301	NAG	C4-C5-C6-O6
5	F	605	NAG	C4-C5-C6-O6
5	F	602	NAG	O5-C5-C6-O6
5	F	602	NAG	C4-C5-C6-O6
5	F	601	NAG	C4-C5-C6-O6
5	F	605	NAG	O5-C5-C6-O6
5	F	601	NAG	O5-C5-C6-O6

There are no ring outliers.

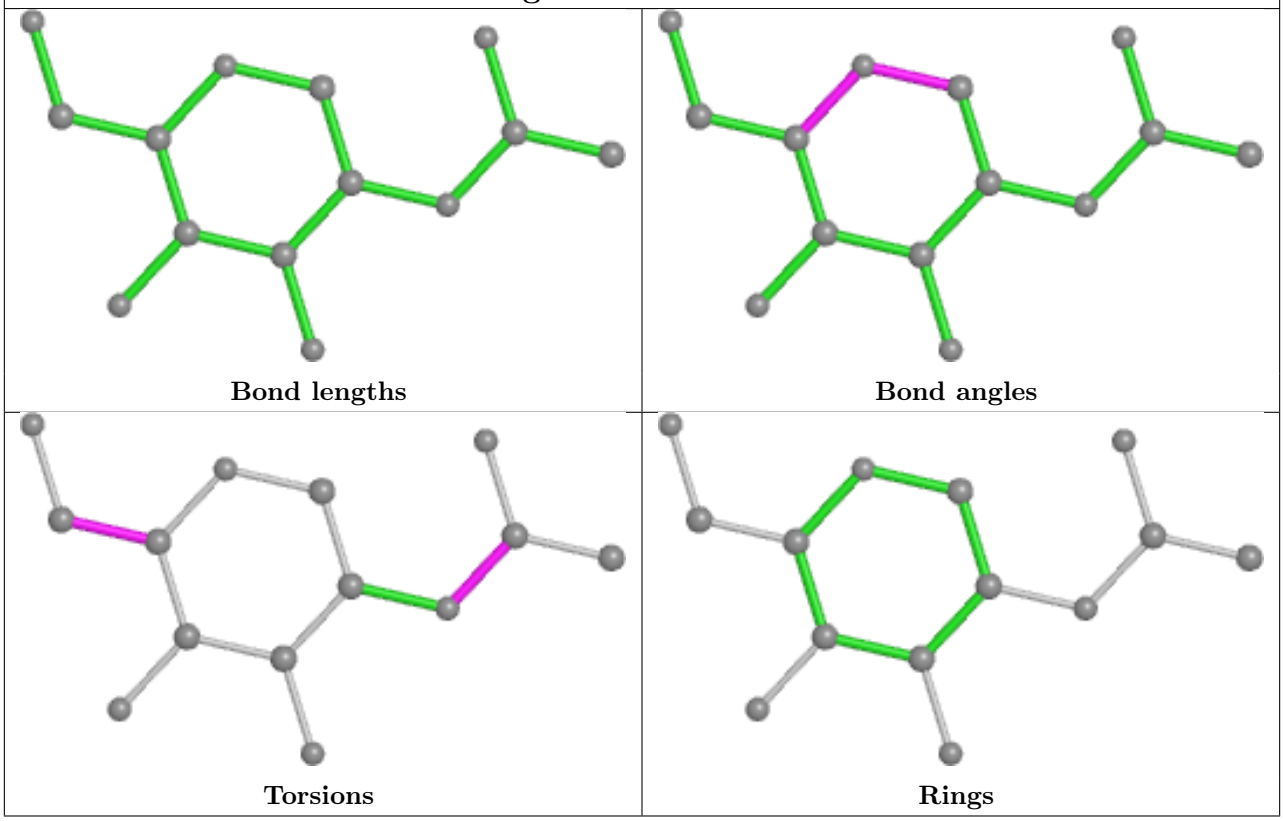
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	605	NAG	1	0

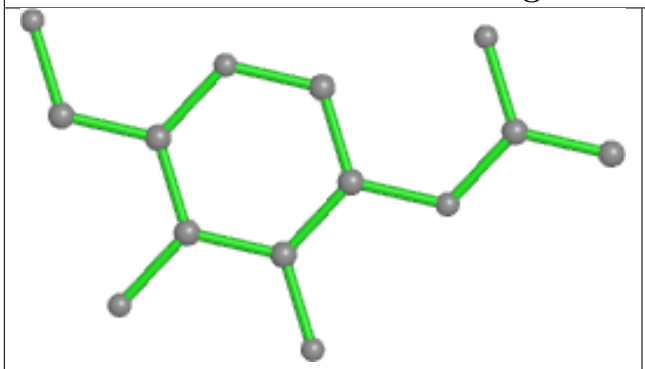
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

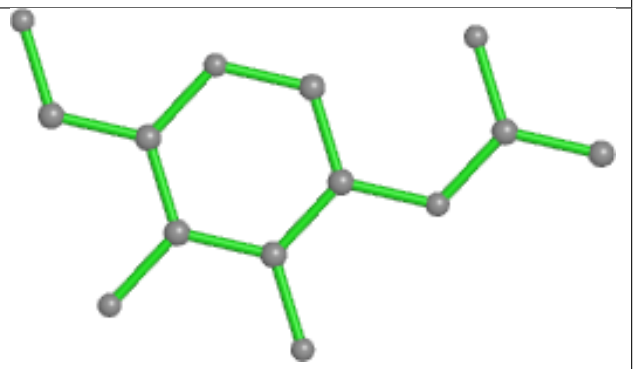
Ligand NAG F 605



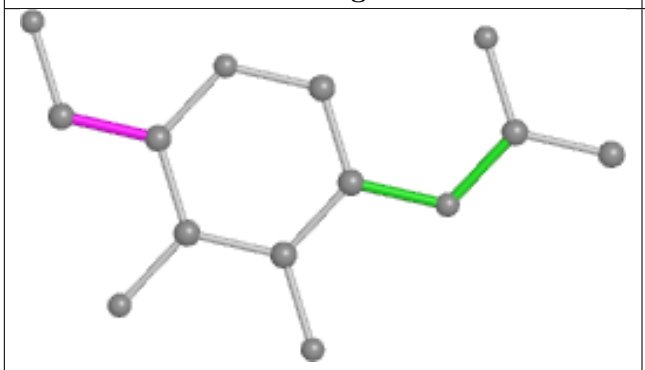
Ligand NAG F 602



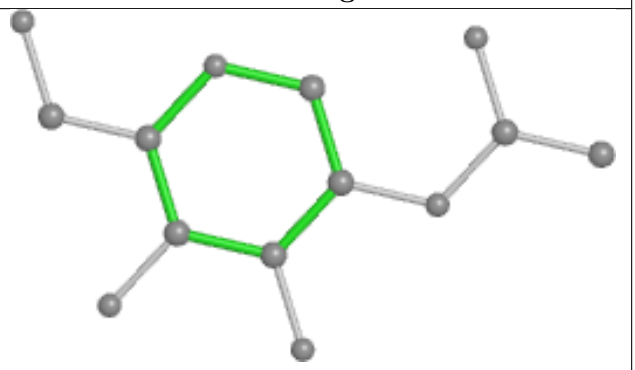
Bond lengths



Bond angles

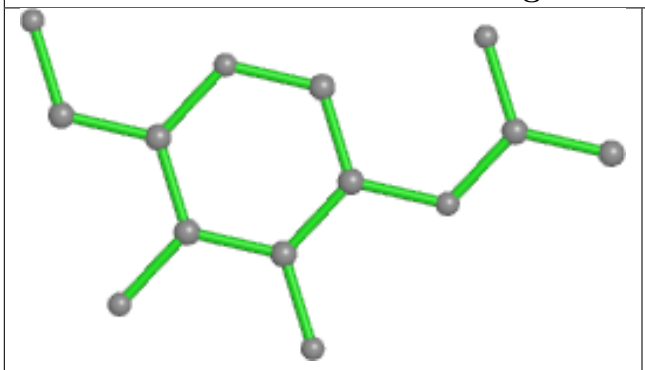


Torsions

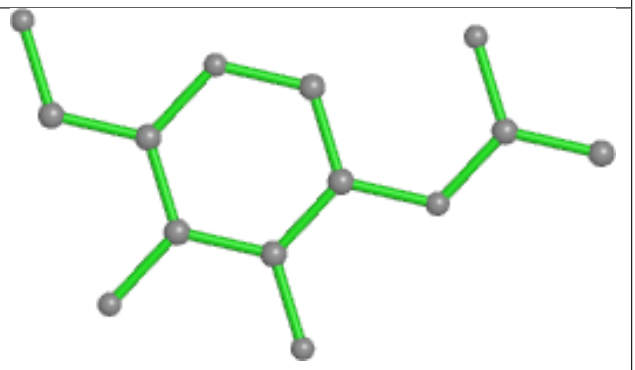


Rings

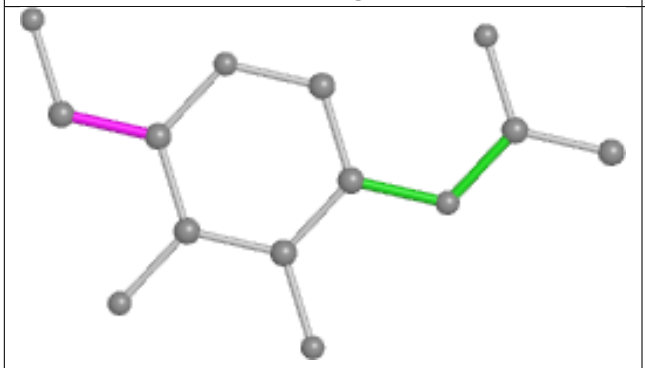
Ligand NAG F 601



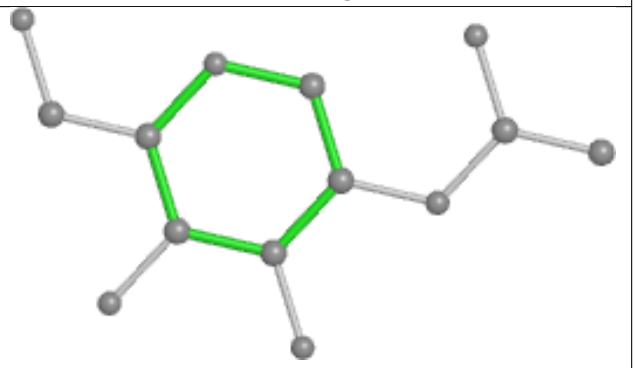
Bond lengths



Bond angles

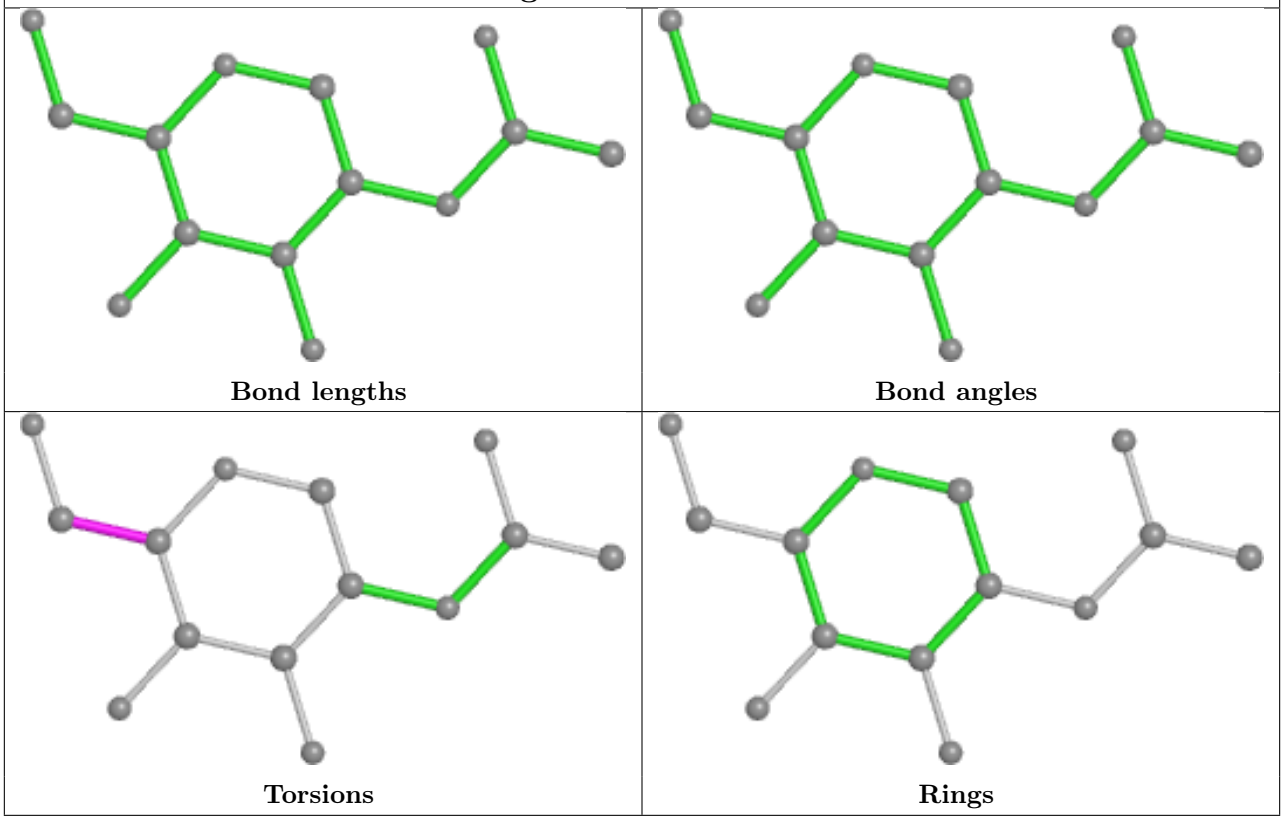


Torsions



Rings

Ligand NAG H 301



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	F	454/502 (90%)	0.56	3 (0%)	87	81	45, 78, 142, 245	0
2	L	215/216 (99%)	1.08	42 (19%)	1	1	75, 127, 229, 293	0
3	H	201/228 (88%)	1.39	57 (28%)	0	0	70, 153, 223, 287	0
All	All	870/946 (91%)	0.88	102 (11%)	4	2	45, 98, 209, 293	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	138	LEU	7.9
3	H	123	PRO	6.7
2	L	119	PRO	5.9
3	H	141	LEU	5.7
2	L	177	THR	5.7
3	H	122	PHE	5.6
2	L	185	TYR	5.5
3	H	124	LEU	5.4
3	H	181	VAL	5.3
3	H	195	VAL	5.2
2	L	133	VAL	5.1
3	H	182	VAL	5.1
3	H	140	CYS	4.9
3	H	112	SER	4.9
3	H	146	LEU	4.7
2	L	132	ILE	4.5
2	L	131	THR	4.4
2	L	153	THR	4.3
3	H	180	SER	4.2
3	H	206	LYS	4.2
2	L	174	LEU	4.2
3	H	125	ALA	4.2
2	L	135	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
2	L	136	ALA	4.1
2	L	120	PRO	4.1
3	H	143	LYS	4.0
2	L	148	GLU	4.0
3	H	126	PRO	4.0
1	F	108	VAL	4.0
2	L	147	TRP	4.0
3	H	152	VAL	4.0
3	H	204	VAL	4.0
2	L	154	GLN	3.9
3	H	142	VAL	3.9
2	L	134	CYS	3.9
2	L	179	THR	3.8
3	H	207	THR	3.8
3	H	121	VAL	3.7
3	H	109	VAL	3.6
3	H	139	GLY	3.6
1	F	107	ASP	3.6
2	L	118	PHE	3.5
2	L	206	PHE	3.4
2	L	193	CYS	3.4
3	H	208	VAL	3.3
2	L	124	GLN	3.3
2	L	180	LEU	3.3
2	L	155	THR	3.3
3	H	170	ARG	3.3
3	H	18	LEU	3.3
3	H	36	TRP	3.3
2	L	145	VAL	3.2
3	H	67	PHE	3.2
2	L	194	LYS	3.2
3	H	82	MET	3.1
3	H	178	LEU	3.0
2	L	178	LEU	3.0
3	H	199	ALA	3.0
2	L	175	SER	3.0
2	L	127	THR	2.9
2	L	203	VAL	2.9
3	H	205	ASP	2.8
2	L	191	TYR	2.8
3	H	137	THR	2.8
3	H	75	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	L	176	SER	2.7
3	H	183	SER	2.7
3	H	110	THR	2.7
2	L	195	VAL	2.6
3	H	113	SER	2.6
2	L	211	CYS	2.5
3	H	179	SER	2.5
3	H	108	LEU	2.4
2	L	115	VAL	2.4
3	H	17	THR	2.4
3	H	90	TYR	2.4
3	H	158	THR	2.4
2	L	130	VAL	2.4
2	L	116	LEU	2.3
3	H	203	LYS	2.3
2	L	95(A)	ILE	2.3
3	H	48	ILE	2.2
3	H	111	VAL	2.2
2	L	161	SER	2.2
3	H	151	THR	2.2
3	H	117	LYS	2.2
2	L	200	THR	2.2
2	L	117	ILE	2.2
2	L	192	THR	2.2
3	H	145	TYR	2.2
1	F	445	ILE	2.1
3	H	153	THR	2.1
3	H	196	ALA	2.1
3	H	91	PHE	2.1
3	H	37	VAL	2.1
3	H	45	LEU	2.1
2	L	97	ALA	2.0
2	L	29	ILE	2.0
3	H	15	GLY	2.0
3	H	119	PRO	2.0
3	H	103	TRP	2.0
3	H	80	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)

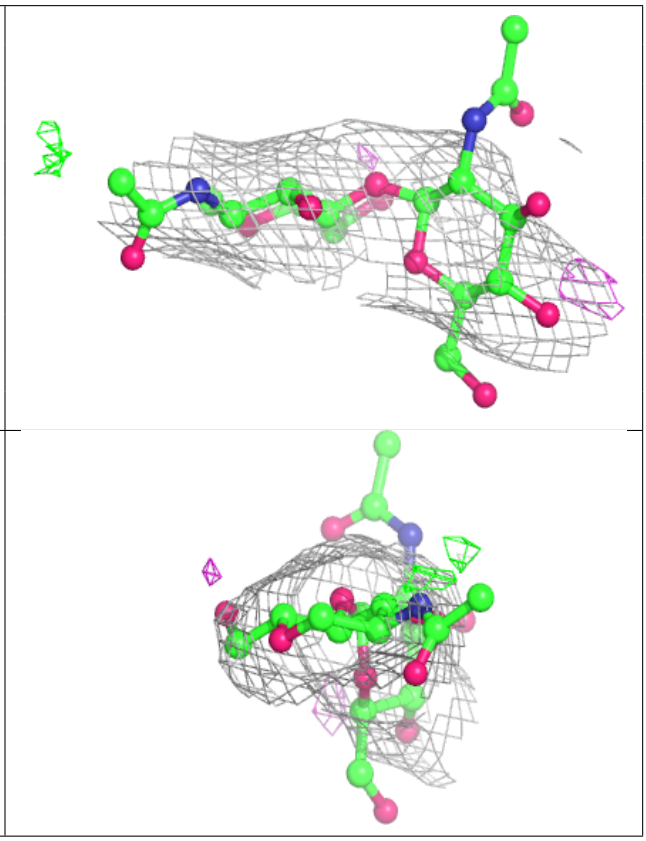
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	2	14/15	0.76	0.38	159,199,205,205	0
4	NAG	A	1	14/15	0.90	0.34	141,157,187,195	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 A:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	H	301	14/15	0.70	0.57	176,198,209,209	0

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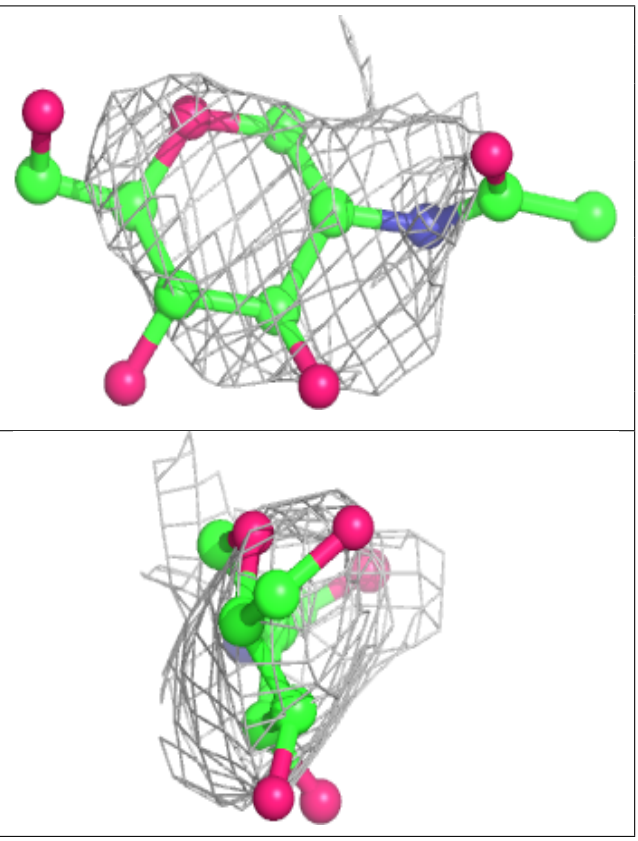
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	F	601	14/15	0.90	0.19	101,132,150,154	0
5	NAG	F	605	14/15	0.92	0.25	68,81,102,127	0
5	NAG	F	602	14/15	0.95	0.23	65,79,94,95	0

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.

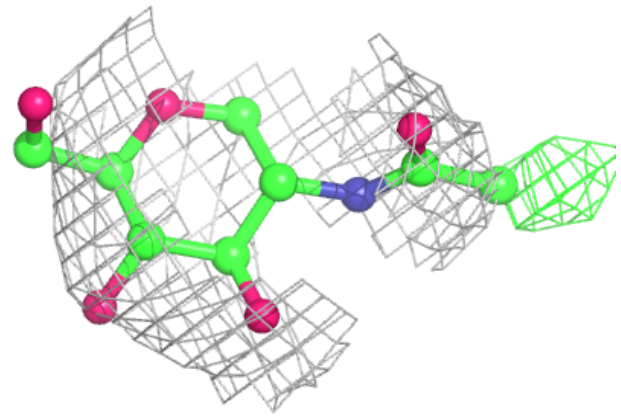
Electron density around NAG H 301:

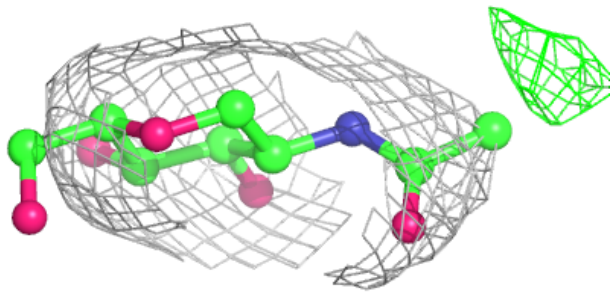
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

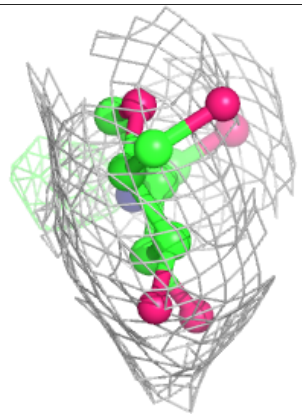


Electron density around NAG F 601:

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

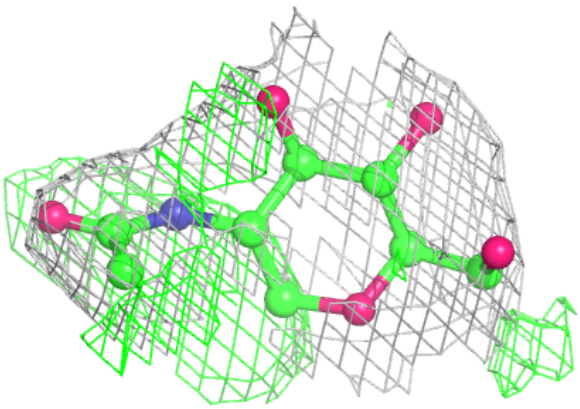


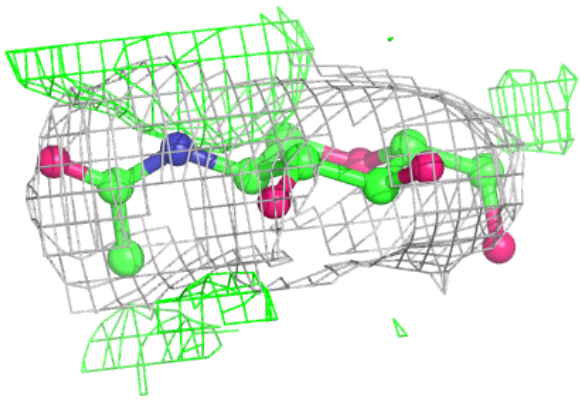


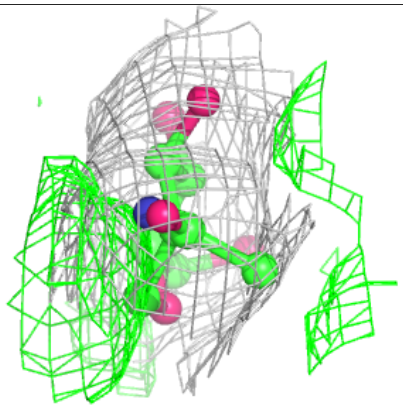


Electron density around NAG F 605:

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

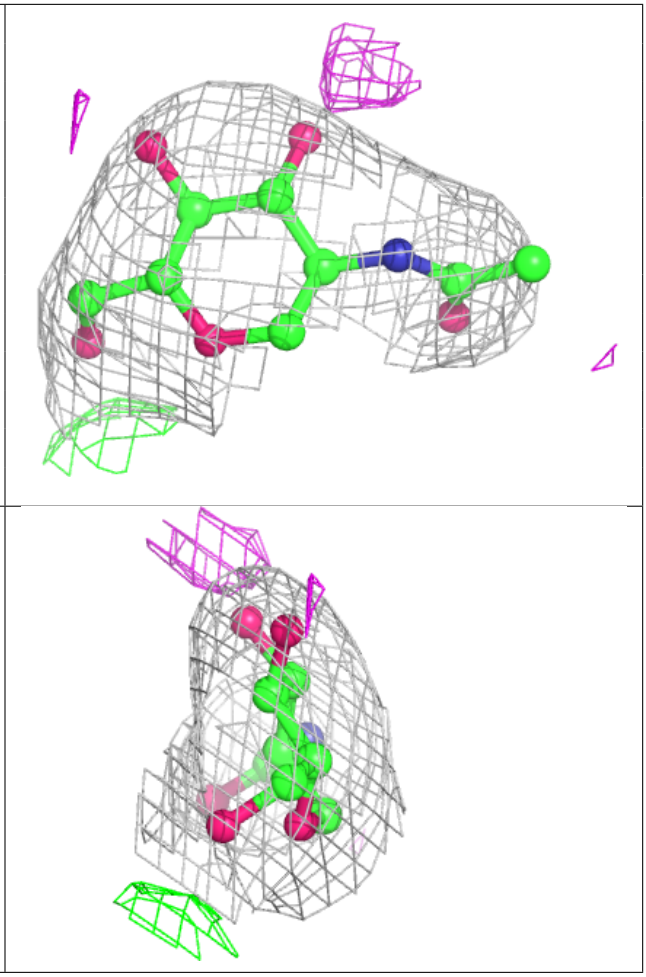






Electron density around NAG F 602:

$2mF_o$-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.