



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:46 AM UTC

PDB ID : 6Z3M / pdb_00006z3m
Title : Repulsive Guidance Molecule B (RGMB) in complex with Growth Differentiation Factor 5 (GDF5) and Neogenin 1 (NEO1).
Authors : Malinauskas, T.; Peer, T.V.; Bishop, B.; Muller, T.D.; Siebold, C.
Deposited on : 2020-05-21
Resolution : 5.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

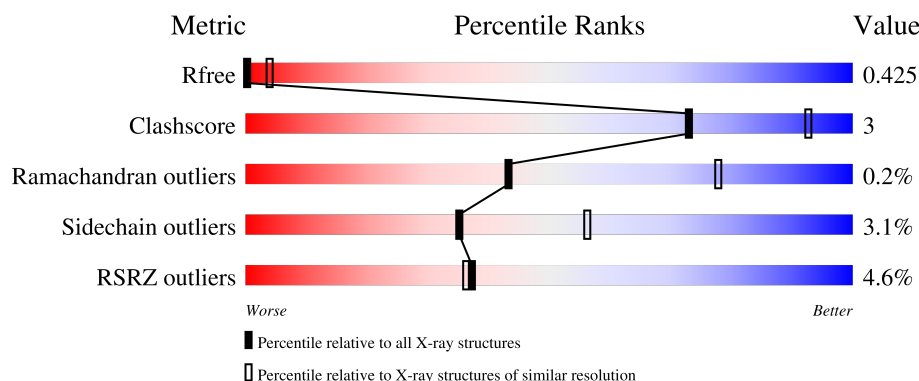
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1088 (7.00-4.00)
Clashscore	190562	1147 (7.00-4.00)
Ramachandran outliers	187476	1012 (7.02-3.98)
Sidechain outliers	187428	1023 (7.04-3.96)
RSRZ outliers	180081	1081 (7.00-4.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	117	3% 84% 5% • 10%
1	B	117	4% 85% 5% • 9%
1	G	117	3% 84% 6% • 9%
1	H	117	3% 86% • • 10%
1	M	117	2% 86% • • 10%

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Mol	Chain	Length	Quality of chain
1	N	117	
2	C	371	
2	D	371	
2	I	371	
2	J	371	
2	O	371	
2	P	371	
2	S	371	
2	T	371	
2	U	371	
2	V	371	
2	W	371	
2	X	371	
2	c	371	
2	d	371	
2	i	371	
2	j	371	
2	o	371	
2	p	371	
3	E	253	
3	F	253	
3	K	253	
3	L	253	
3	Q	253	
3	R	253	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25210 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 Growth/differentiation factor 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	0	0	0
			813	508	140	154	11			
1	B	106	Total	C	N	O	S	0	0	0
			828	520	141	156	11			
1	G	106	Total	C	N	O	S	0	0	0
			821	514	141	155	11			
1	H	105	Total	C	N	O	S	0	0	0
			811	506	140	154	11			
1	M	105	Total	C	N	O	S	0	0	0
			813	507	140	155	11			
1	N	106	Total	C	N	O	S	0	0	0
			831	522	142	156	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	385	MET	-	initiating methionine	UNP P43026
A	386	LYS	-	expression tag	UNP P43026
B	385	MET	-	initiating methionine	UNP P43026
B	386	LYS	-	expression tag	UNP P43026
G	385	MET	-	initiating methionine	UNP P43026
G	386	LYS	-	expression tag	UNP P43026
H	385	MET	-	initiating methionine	UNP P43026
H	386	LYS	-	expression tag	UNP P43026
M	385	MET	-	initiating methionine	UNP P43026
M	386	LYS	-	expression tag	UNP P43026
N	385	MET	-	initiating methionine	UNP P43026
N	386	LYS	-	expression tag	UNP P43026

- Molecule 2 is a protein called RGM domain family member B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	74	Total	C	N	O	S	0	0	0
			556	336	104	109	7			
2	D	75	Total	C	N	O	S	0	0	0
			566	343	105	111	7			
2	I	71	Total	C	N	O	S	0	0	0
			536	326	100	103	7			
2	J	73	Total	C	N	O	S	0	0	0
			522	313	99	103	7			
2	O	71	Total	C	N	O	S	0	0	0
			529	321	97	104	7			
2	P	76	Total	C	N	O	S	0	0	0
			570	345	106	112	7			
2	c	158	Total	C	N	O	S	0	0	0
			1218	771	204	235	8			
2	d	158	Total	C	N	O	S	0	0	0
			1219	772	204	235	8			
2	i	158	Total	C	N	O	S	0	0	0
			1193	753	198	234	8			
2	j	158	Total	C	N	O	S	0	0	0
			1211	767	201	235	8			
2	o	158	Total	C	N	O	S	0	0	0
			1207	766	198	235	8			
2	p	158	Total	C	N	O	S	0	0	0
			1212	767	204	233	8			
2	S	4	Total	C	N	O	S	0	0	0
			33	21	5	6	1			
2	T	4	Total	C	N	O	S	0	0	0
			33	21	5	6	1			
2	U	4	Total	C	N	O	S	0	0	0
			33	21	5	6	1			
2	V	4	Total	C	N	O	S	0	0	0
			33	21	5	6	1			
2	W	4	Total	C	N	O	S	0	0	0
			33	21	5	6	1			
2	X	4	Total	C	N	O	S	0	0	0
			33	21	5	6	1			

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	50	GLU	-	expression tag	UNP Q6NW40
C	51	THR	-	expression tag	UNP Q6NW40
C	52	GLY	-	expression tag	UNP Q6NW40
C	225	GLY	GLU	conflict	UNP Q6NW40

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Chain	Residue	Modelled	Actual	Comment	Reference
C	413	THR	-	expression tag	UNP Q6NW40
C	414	LYS	-	expression tag	UNP Q6NW40
C	415	HIS	-	expression tag	UNP Q6NW40
C	416	HIS	-	expression tag	UNP Q6NW40
C	417	HIS	-	expression tag	UNP Q6NW40
C	418	HIS	-	expression tag	UNP Q6NW40
C	419	HIS	-	expression tag	UNP Q6NW40
C	420	HIS	-	expression tag	UNP Q6NW40
D	50	GLU	-	expression tag	UNP Q6NW40
D	51	THR	-	expression tag	UNP Q6NW40
D	52	GLY	-	expression tag	UNP Q6NW40
D	225	GLY	GLU	conflict	UNP Q6NW40
D	413	THR	-	expression tag	UNP Q6NW40
D	414	LYS	-	expression tag	UNP Q6NW40
D	415	HIS	-	expression tag	UNP Q6NW40
D	416	HIS	-	expression tag	UNP Q6NW40
D	417	HIS	-	expression tag	UNP Q6NW40
D	418	HIS	-	expression tag	UNP Q6NW40
D	419	HIS	-	expression tag	UNP Q6NW40
D	420	HIS	-	expression tag	UNP Q6NW40
I	50	GLU	-	expression tag	UNP Q6NW40
I	51	THR	-	expression tag	UNP Q6NW40
I	52	GLY	-	expression tag	UNP Q6NW40
I	225	GLY	GLU	conflict	UNP Q6NW40
I	413	THR	-	expression tag	UNP Q6NW40
I	414	LYS	-	expression tag	UNP Q6NW40
I	415	HIS	-	expression tag	UNP Q6NW40
I	416	HIS	-	expression tag	UNP Q6NW40
I	417	HIS	-	expression tag	UNP Q6NW40
I	418	HIS	-	expression tag	UNP Q6NW40
I	419	HIS	-	expression tag	UNP Q6NW40
I	420	HIS	-	expression tag	UNP Q6NW40
J	50	GLU	-	expression tag	UNP Q6NW40
J	51	THR	-	expression tag	UNP Q6NW40
J	52	GLY	-	expression tag	UNP Q6NW40
J	225	GLY	GLU	conflict	UNP Q6NW40
J	413	THR	-	expression tag	UNP Q6NW40
J	414	LYS	-	expression tag	UNP Q6NW40
J	415	HIS	-	expression tag	UNP Q6NW40
J	416	HIS	-	expression tag	UNP Q6NW40
J	417	HIS	-	expression tag	UNP Q6NW40
J	418	HIS	-	expression tag	UNP Q6NW40

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Chain	Residue	Modelled	Actual	Comment	Reference
J	419	HIS	-	expression tag	UNP Q6NW40
J	420	HIS	-	expression tag	UNP Q6NW40
O	50	GLU	-	expression tag	UNP Q6NW40
O	51	THR	-	expression tag	UNP Q6NW40
O	52	GLY	-	expression tag	UNP Q6NW40
O	225	GLY	GLU	conflict	UNP Q6NW40
O	413	THR	-	expression tag	UNP Q6NW40
O	414	LYS	-	expression tag	UNP Q6NW40
O	415	HIS	-	expression tag	UNP Q6NW40
O	416	HIS	-	expression tag	UNP Q6NW40
O	417	HIS	-	expression tag	UNP Q6NW40
O	418	HIS	-	expression tag	UNP Q6NW40
O	419	HIS	-	expression tag	UNP Q6NW40
O	420	HIS	-	expression tag	UNP Q6NW40
P	50	GLU	-	expression tag	UNP Q6NW40
P	51	THR	-	expression tag	UNP Q6NW40
P	52	GLY	-	expression tag	UNP Q6NW40
P	225	GLY	GLU	conflict	UNP Q6NW40
P	413	THR	-	expression tag	UNP Q6NW40
P	414	LYS	-	expression tag	UNP Q6NW40
P	415	HIS	-	expression tag	UNP Q6NW40
P	416	HIS	-	expression tag	UNP Q6NW40
P	417	HIS	-	expression tag	UNP Q6NW40
P	418	HIS	-	expression tag	UNP Q6NW40
P	419	HIS	-	expression tag	UNP Q6NW40
P	420	HIS	-	expression tag	UNP Q6NW40
c	50	GLU	-	expression tag	UNP Q6NW40
c	51	THR	-	expression tag	UNP Q6NW40
c	52	GLY	-	expression tag	UNP Q6NW40
c	225	GLY	GLU	conflict	UNP Q6NW40
c	413	THR	-	expression tag	UNP Q6NW40
c	414	LYS	-	expression tag	UNP Q6NW40
c	415	HIS	-	expression tag	UNP Q6NW40
c	416	HIS	-	expression tag	UNP Q6NW40
c	417	HIS	-	expression tag	UNP Q6NW40
c	418	HIS	-	expression tag	UNP Q6NW40
c	419	HIS	-	expression tag	UNP Q6NW40
c	420	HIS	-	expression tag	UNP Q6NW40
d	50	GLU	-	expression tag	UNP Q6NW40
d	51	THR	-	expression tag	UNP Q6NW40
d	52	GLY	-	expression tag	UNP Q6NW40
d	225	GLY	GLU	conflict	UNP Q6NW40

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Chain	Residue	Modelled	Actual	Comment	Reference
d	413	THR	-	expression tag	UNP Q6NW40
d	414	LYS	-	expression tag	UNP Q6NW40
d	415	HIS	-	expression tag	UNP Q6NW40
d	416	HIS	-	expression tag	UNP Q6NW40
d	417	HIS	-	expression tag	UNP Q6NW40
d	418	HIS	-	expression tag	UNP Q6NW40
d	419	HIS	-	expression tag	UNP Q6NW40
d	420	HIS	-	expression tag	UNP Q6NW40
i	50	GLU	-	expression tag	UNP Q6NW40
i	51	THR	-	expression tag	UNP Q6NW40
i	52	GLY	-	expression tag	UNP Q6NW40
i	225	GLY	GLU	conflict	UNP Q6NW40
i	413	THR	-	expression tag	UNP Q6NW40
i	414	LYS	-	expression tag	UNP Q6NW40
i	415	HIS	-	expression tag	UNP Q6NW40
i	416	HIS	-	expression tag	UNP Q6NW40
i	417	HIS	-	expression tag	UNP Q6NW40
i	418	HIS	-	expression tag	UNP Q6NW40
i	419	HIS	-	expression tag	UNP Q6NW40
i	420	HIS	-	expression tag	UNP Q6NW40
j	50	GLU	-	expression tag	UNP Q6NW40
j	51	THR	-	expression tag	UNP Q6NW40
j	52	GLY	-	expression tag	UNP Q6NW40
j	225	GLY	GLU	conflict	UNP Q6NW40
j	413	THR	-	expression tag	UNP Q6NW40
j	414	LYS	-	expression tag	UNP Q6NW40
j	415	HIS	-	expression tag	UNP Q6NW40
j	416	HIS	-	expression tag	UNP Q6NW40
j	417	HIS	-	expression tag	UNP Q6NW40
j	418	HIS	-	expression tag	UNP Q6NW40
j	419	HIS	-	expression tag	UNP Q6NW40
j	420	HIS	-	expression tag	UNP Q6NW40
o	50	GLU	-	expression tag	UNP Q6NW40
o	51	THR	-	expression tag	UNP Q6NW40
o	52	GLY	-	expression tag	UNP Q6NW40
o	225	GLY	GLU	conflict	UNP Q6NW40
o	413	THR	-	expression tag	UNP Q6NW40
o	414	LYS	-	expression tag	UNP Q6NW40
o	415	HIS	-	expression tag	UNP Q6NW40
o	416	HIS	-	expression tag	UNP Q6NW40
o	417	HIS	-	expression tag	UNP Q6NW40
o	418	HIS	-	expression tag	UNP Q6NW40

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Chain	Residue	Modelled	Actual	Comment	Reference
o	419	HIS	-	expression tag	UNP Q6NW40
o	420	HIS	-	expression tag	UNP Q6NW40
p	50	GLU	-	expression tag	UNP Q6NW40
p	51	THR	-	expression tag	UNP Q6NW40
p	52	GLY	-	expression tag	UNP Q6NW40
p	225	GLY	GLU	conflict	UNP Q6NW40
p	413	THR	-	expression tag	UNP Q6NW40
p	414	LYS	-	expression tag	UNP Q6NW40
p	415	HIS	-	expression tag	UNP Q6NW40
p	416	HIS	-	expression tag	UNP Q6NW40
p	417	HIS	-	expression tag	UNP Q6NW40
p	418	HIS	-	expression tag	UNP Q6NW40
p	419	HIS	-	expression tag	UNP Q6NW40
p	420	HIS	-	expression tag	UNP Q6NW40
S	50	GLU	-	expression tag	UNP Q6NW40
S	51	THR	-	expression tag	UNP Q6NW40
S	52	GLY	-	expression tag	UNP Q6NW40
S	225	GLY	GLU	conflict	UNP Q6NW40
S	413	THR	-	expression tag	UNP Q6NW40
S	414	LYS	-	expression tag	UNP Q6NW40
S	415	HIS	-	expression tag	UNP Q6NW40
S	416	HIS	-	expression tag	UNP Q6NW40
S	417	HIS	-	expression tag	UNP Q6NW40
S	418	HIS	-	expression tag	UNP Q6NW40
S	419	HIS	-	expression tag	UNP Q6NW40
S	420	HIS	-	expression tag	UNP Q6NW40
T	50	GLU	-	expression tag	UNP Q6NW40
T	51	THR	-	expression tag	UNP Q6NW40
T	52	GLY	-	expression tag	UNP Q6NW40
T	225	GLY	GLU	conflict	UNP Q6NW40
T	413	THR	-	expression tag	UNP Q6NW40
T	414	LYS	-	expression tag	UNP Q6NW40
T	415	HIS	-	expression tag	UNP Q6NW40
T	416	HIS	-	expression tag	UNP Q6NW40
T	417	HIS	-	expression tag	UNP Q6NW40
T	418	HIS	-	expression tag	UNP Q6NW40
T	419	HIS	-	expression tag	UNP Q6NW40
T	420	HIS	-	expression tag	UNP Q6NW40
U	50	GLU	-	expression tag	UNP Q6NW40
U	51	THR	-	expression tag	UNP Q6NW40
U	52	GLY	-	expression tag	UNP Q6NW40
U	225	GLY	GLU	conflict	UNP Q6NW40

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Chain	Residue	Modelled	Actual	Comment	Reference
U	413	THR	-	expression tag	UNP Q6NW40
U	414	LYS	-	expression tag	UNP Q6NW40
U	415	HIS	-	expression tag	UNP Q6NW40
U	416	HIS	-	expression tag	UNP Q6NW40
U	417	HIS	-	expression tag	UNP Q6NW40
U	418	HIS	-	expression tag	UNP Q6NW40
U	419	HIS	-	expression tag	UNP Q6NW40
U	420	HIS	-	expression tag	UNP Q6NW40
V	50	GLU	-	expression tag	UNP Q6NW40
V	51	THR	-	expression tag	UNP Q6NW40
V	52	GLY	-	expression tag	UNP Q6NW40
V	225	GLY	GLU	conflict	UNP Q6NW40
V	413	THR	-	expression tag	UNP Q6NW40
V	414	LYS	-	expression tag	UNP Q6NW40
V	415	HIS	-	expression tag	UNP Q6NW40
V	416	HIS	-	expression tag	UNP Q6NW40
V	417	HIS	-	expression tag	UNP Q6NW40
V	418	HIS	-	expression tag	UNP Q6NW40
V	419	HIS	-	expression tag	UNP Q6NW40
V	420	HIS	-	expression tag	UNP Q6NW40
W	50	GLU	-	expression tag	UNP Q6NW40
W	51	THR	-	expression tag	UNP Q6NW40
W	52	GLY	-	expression tag	UNP Q6NW40
W	225	GLY	GLU	conflict	UNP Q6NW40
W	413	THR	-	expression tag	UNP Q6NW40
W	414	LYS	-	expression tag	UNP Q6NW40
W	415	HIS	-	expression tag	UNP Q6NW40
W	416	HIS	-	expression tag	UNP Q6NW40
W	417	HIS	-	expression tag	UNP Q6NW40
W	418	HIS	-	expression tag	UNP Q6NW40
W	419	HIS	-	expression tag	UNP Q6NW40
W	420	HIS	-	expression tag	UNP Q6NW40
X	50	GLU	-	expression tag	UNP Q6NW40
X	51	THR	-	expression tag	UNP Q6NW40
X	52	GLY	-	expression tag	UNP Q6NW40
X	225	GLY	GLU	conflict	UNP Q6NW40
X	413	THR	-	expression tag	UNP Q6NW40
X	414	LYS	-	expression tag	UNP Q6NW40
X	415	HIS	-	expression tag	UNP Q6NW40
X	416	HIS	-	expression tag	UNP Q6NW40
X	417	HIS	-	expression tag	UNP Q6NW40
X	418	HIS	-	expression tag	UNP Q6NW40

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Chain	Residue	Modelled	Actual	Comment	Reference
X	419	HIS	-	expression tag	UNP Q6NW40
X	420	HIS	-	expression tag	UNP Q6NW40

- Molecule 3 is a protein called Neogenin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	205	Total	C	N	O	S	0	0	0
			1602	1022	272	302	6			
3	F	205	Total	C	N	O	S	0	0	0
			1596	1018	270	302	6			
3	K	205	Total	C	N	O	S	0	0	0
			1604	1025	271	302	6			
3	L	187	Total	C	N	O	S	0	0	0
			1429	915	243	265	6			
3	Q	205	Total	C	N	O	S	0	0	0
			1603	1024	271	302	6			
3	R	205	Total	C	N	O	S	0	0	0
			1596	1019	269	302	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	880	GLU	-	expression tag	UNP P97798
E	881	THR	-	expression tag	UNP P97798
E	882	GLY	-	expression tag	UNP P97798
E	1124	GLY	-	expression tag	UNP P97798
E	1125	THR	-	expression tag	UNP P97798
E	1126	LYS	-	expression tag	UNP P97798
E	1127	HIS	-	expression tag	UNP P97798
E	1128	HIS	-	expression tag	UNP P97798
E	1129	HIS	-	expression tag	UNP P97798
E	1130	HIS	-	expression tag	UNP P97798
E	1131	HIS	-	expression tag	UNP P97798
E	1132	HIS	-	expression tag	UNP P97798
F	880	GLU	-	expression tag	UNP P97798
F	881	THR	-	expression tag	UNP P97798
F	882	GLY	-	expression tag	UNP P97798
F	1124	GLY	-	expression tag	UNP P97798
F	1125	THR	-	expression tag	UNP P97798
F	1126	LYS	-	expression tag	UNP P97798
F	1127	HIS	-	expression tag	UNP P97798
F	1128	HIS	-	expression tag	UNP P97798

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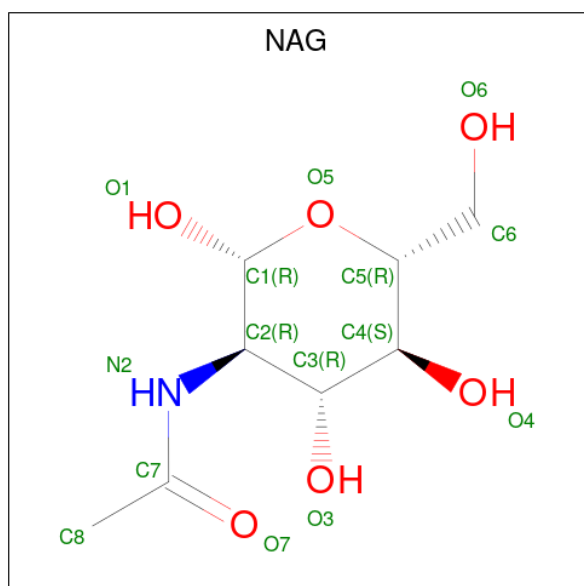
Chain	Residue	Modelled	Actual	Comment	Reference
F	1129	HIS	-	expression tag	UNP P97798
F	1130	HIS	-	expression tag	UNP P97798
F	1131	HIS	-	expression tag	UNP P97798
F	1132	HIS	-	expression tag	UNP P97798
K	880	GLU	-	expression tag	UNP P97798
K	881	THR	-	expression tag	UNP P97798
K	882	GLY	-	expression tag	UNP P97798
K	1124	GLY	-	expression tag	UNP P97798
K	1125	THR	-	expression tag	UNP P97798
K	1126	LYS	-	expression tag	UNP P97798
K	1127	HIS	-	expression tag	UNP P97798
K	1128	HIS	-	expression tag	UNP P97798
K	1129	HIS	-	expression tag	UNP P97798
K	1130	HIS	-	expression tag	UNP P97798
K	1131	HIS	-	expression tag	UNP P97798
K	1132	HIS	-	expression tag	UNP P97798
L	880	GLU	-	expression tag	UNP P97798
L	881	THR	-	expression tag	UNP P97798
L	882	GLY	-	expression tag	UNP P97798
L	1124	GLY	-	expression tag	UNP P97798
L	1125	THR	-	expression tag	UNP P97798
L	1126	LYS	-	expression tag	UNP P97798
L	1127	HIS	-	expression tag	UNP P97798
L	1128	HIS	-	expression tag	UNP P97798
L	1129	HIS	-	expression tag	UNP P97798
L	1130	HIS	-	expression tag	UNP P97798
L	1131	HIS	-	expression tag	UNP P97798
L	1132	HIS	-	expression tag	UNP P97798
Q	880	GLU	-	expression tag	UNP P97798
Q	881	THR	-	expression tag	UNP P97798
Q	882	GLY	-	expression tag	UNP P97798
Q	1124	GLY	-	expression tag	UNP P97798
Q	1125	THR	-	expression tag	UNP P97798
Q	1126	LYS	-	expression tag	UNP P97798
Q	1127	HIS	-	expression tag	UNP P97798
Q	1128	HIS	-	expression tag	UNP P97798
Q	1129	HIS	-	expression tag	UNP P97798
Q	1130	HIS	-	expression tag	UNP P97798
Q	1131	HIS	-	expression tag	UNP P97798
Q	1132	HIS	-	expression tag	UNP P97798
R	880	GLU	-	expression tag	UNP P97798
R	881	THR	-	expression tag	UNP P97798

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Chain	Residue	Modelled	Actual	Comment	Reference
R	882	GLY	-	expression tag	UNP P97798
R	1124	GLY	-	expression tag	UNP P97798
R	1125	THR	-	expression tag	UNP P97798
R	1126	LYS	-	expression tag	UNP P97798
R	1127	HIS	-	expression tag	UNP P97798
R	1128	HIS	-	expression tag	UNP P97798
R	1129	HIS	-	expression tag	UNP P97798
R	1130	HIS	-	expression tag	UNP P97798
R	1131	HIS	-	expression tag	UNP P97798
R	1132	HIS	-	expression tag	UNP P97798

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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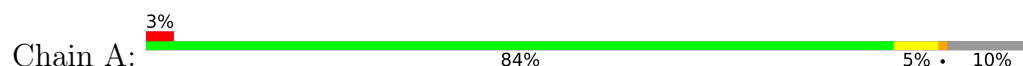
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	P	1	Total	C	N	O	0	0
			14	8	1	5		
4	Q	1	Total	C	N	O	0	0
			14	8	1	5		
4	R	1	Total	C	N	O	0	0
			14	8	1	5		

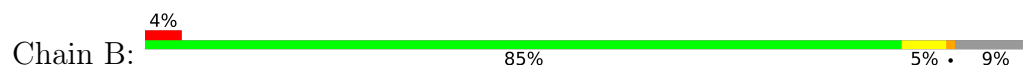
3 Residue-property plots [i](#)

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.

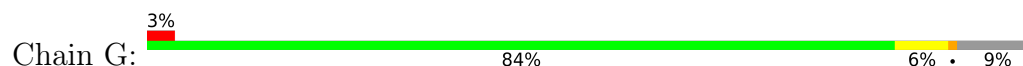
- Molecule 1: Growth/differentiation factor 5



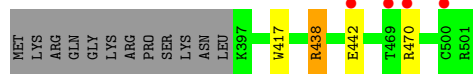
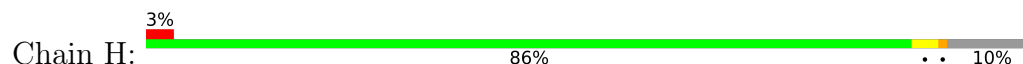
- Molecule 1: Growth/differentiation factor 5



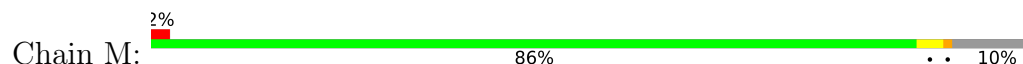
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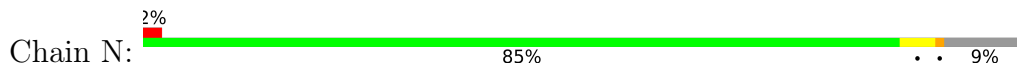
- Molecule 1: Growth/differentiation factor 5



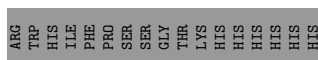
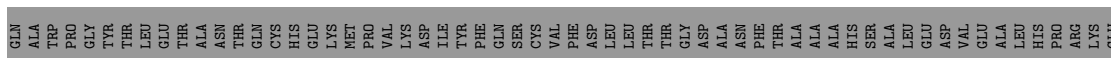
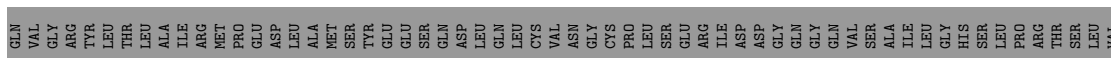
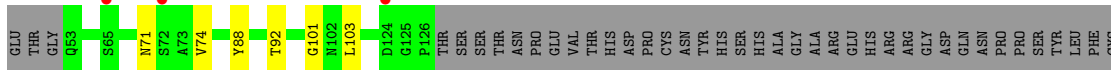
- Molecule 1: Growth/differentiation factor 5



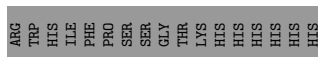
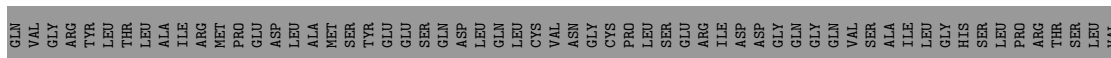
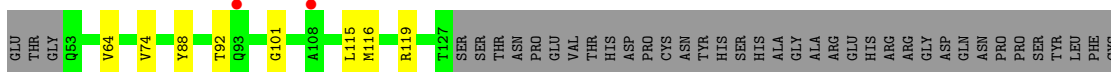
- Molecule 1: Growth/differentiation factor 5



- Molecule 2: RGM domain family member B

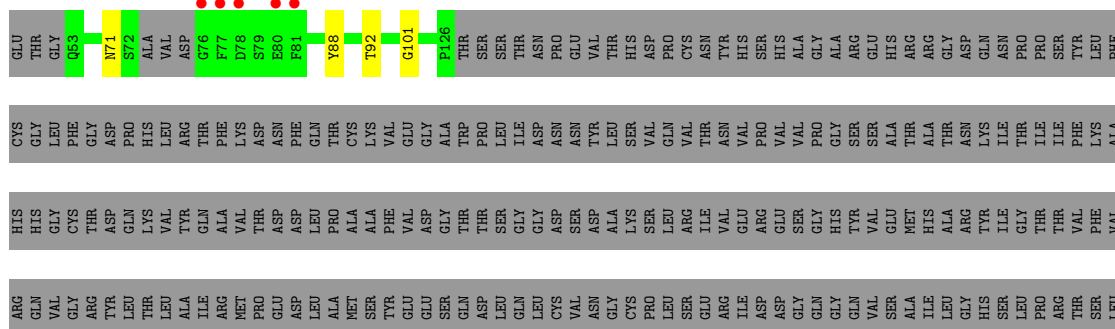


- Molecule 2: RGM domain family member B



- Molecule 2: RGM domain family member B





- Molecule 2: RGM domain family member B

[illegible]

- Molecule 2: RGM domain family member B

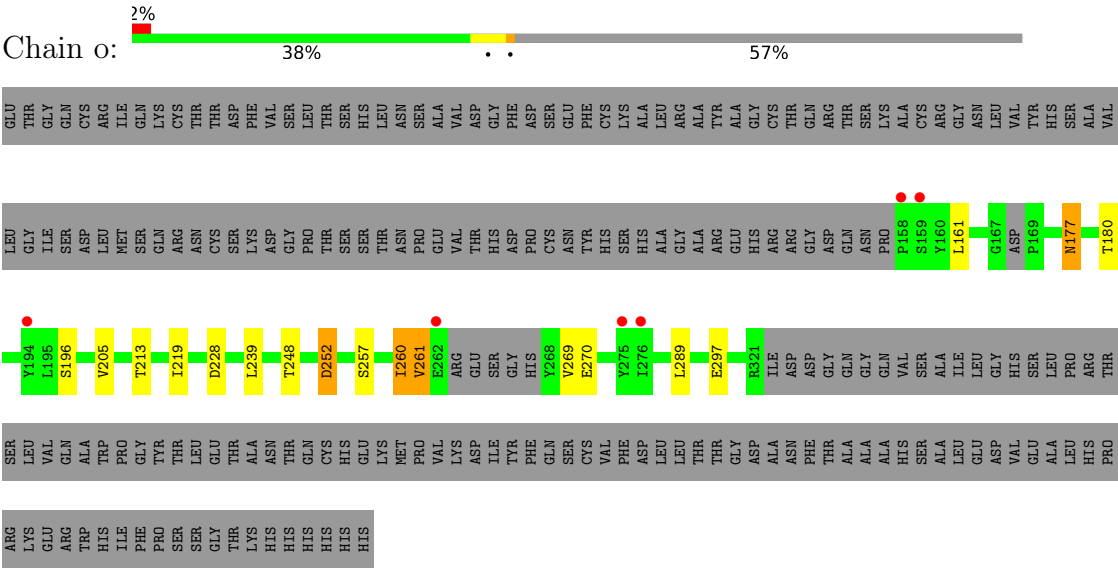


Lys	Leu	N177	Leu	Leu
Glut	Val	F178	Gly	Gly
Arg	Gln		Ile	Ile
Trp	Ala	S196	Ser	Ser
His	Trp		Asp	Asp
Ile	Pro	V205	Leu	Leu
Phe	Gly		Met	Met
Pro	Tyr	T213	Gln	Gln
Ser	Thr		Arg	Arg
Ser	Leu	I219	Asn	Cys
Gly	Glut		Cys	Thr
Thr	Thr	D228	Asn	Thr
Lys	Ala		Ser	Asp
His	Asn	L239	Phe	Ser
His	Thr		Lys	Val
His	Gln	T248	Gly	Ser
His	Cys		Pro	Leu
His	His	D252	Thr	Thr
His	Glut		Ser	Ser
	Lys	S257	Ser	His
	Met		Thr	Leu
	Pro	I260	Asn	Asn
	Val	V261	Pro	Asn
	Lys	E262	Glut	Ser
	Asp	Arg	Val	Ala
	Ile		Thr	Val
	Tyr	Ser	His	Ala
	Phe	Gly	His	Gly
	Gln	His	Pro	Asp
	Ser	Y268	Cys	Ser
	Cys	V269	Asn	Ser
	Val	E270	Tyr	Glut
	Phe		His	Phe
	Asp	L289	Ser	Cys
	Leu		His	Lys
	Leu	R294	Ala	Ala
	Thr		Gly	Leu
	Thr	E297	Ala	Arg
	Gly		Arg	Ala
	Asp	R321	Glut	Tyr
	Ala	Ile	His	Ala
	Asn	Asp	His	Gly
	Phe	Asp	Arg	Cys
	Thr	Gly	Arg	Thr
	Ala	Gln	Gly	Thr
	Ala	Gly	Asp	Arg
	Ala	Gln	Gln	Thr
	His	Val	Asn	Ser
	Ser	Ser	Pro	Lys
	Leu	Ser	F158	Ala
	Leu	Ile	L161	Cys
	Glut	Leu	F162	Arg
	Asp	Gly	G167	Gly
	Val	His	Ser	Asn
	Glut	Ser	Asp	Leu
	Ala	Leu	P169	Val
	Leu	Pro	P172	His
	His	Arg	R172	Ser
	Pro	Thr	S175	Ala
	Arg	Ser		Val

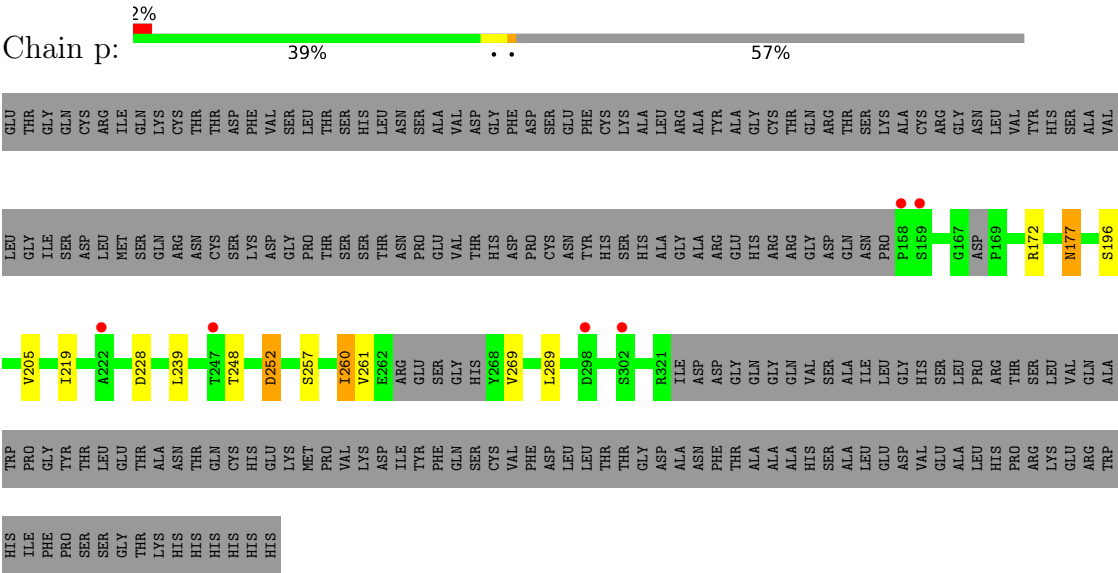
- Molecule 2: RGM domain family member B



GLU	THR	GLY	THR	GLN	GLN	CYS	ARG	ILE	GLN	CYS	LYS	THR	THR	ASP	PHE	VAL	LEU	LEU	ASN	SER	LEU	THR	THR	SER	HIS	LEU	LEU	ASN	ALA	VAL	GLY	ASP	PHE	LYS	CYS	GLY	GLY	CYS	THR	THR	GLN	ARG	THR	THR	SER	LYS	ALA	ALA	ARG	GLY	ASN	LEU	VAL	THR	HIS	SER	ALA	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



● Molecule 2: RGM domain family member B



● Molecule 2: RGM domain family member B



LEU	LEU
GLY	THR
THR	THR
LYS	ALA
HIS	ASN
HIS	ARG
HIS	MET
HIS	PRO
HIS	GLU
HIS	ASP
HIS	ASP
HIS	LEU
HIS	ALA
HIS	MET
HIS	SER
HIS	TYR
HIS	GLU
HIS	GLU
HIS	GLY
HIS	GLN
HIS	ASP
HIS	LEU
HIS	GLN
HIS	GLN
HIS	LEU
HIS	CYS
HIS	VAL
HIS	VAL
HIS	ASN
HIS	GLY
HIS	CYS
HIS	PRO
HIS	LEU
HIS	LEU
HIS	SER
HIS	SER
HIS	GLU
HIS	ARG
HIS	ILE
HIS	ILE
HIS	ASP
HIS	ASP
HIS	GLY
HIS	GLN
HIS	GLN
HIS	GLN
HIS	VAL
HIS	SER
HIS	SER
HIS	ALA
HIS	ALA
HIS	LEU
HIS	LEU
HIS	GLU
HIS	ASP
HIS	ASP
HIS	VAL
HIS	GLU
HIS	ALA
HIS	LEU
HIS	HIS
HIS	HIS
HIS	ARG
HIS	LYS
HIS	GLY
HIS	VAL
HIS	GLN
HIS	GLN
HIS	ALA
HIS	TRP
HIS	TRP
HIS	ILE
HIS	PHE
HIS	PHE
HIS	PRO
HIS	SER

- Molecule 2: RGM domain family member B

Chain T: 99%

[illegible]

- Molecule 2: RGM domain family member B

Chain U: 99%

[illegible]

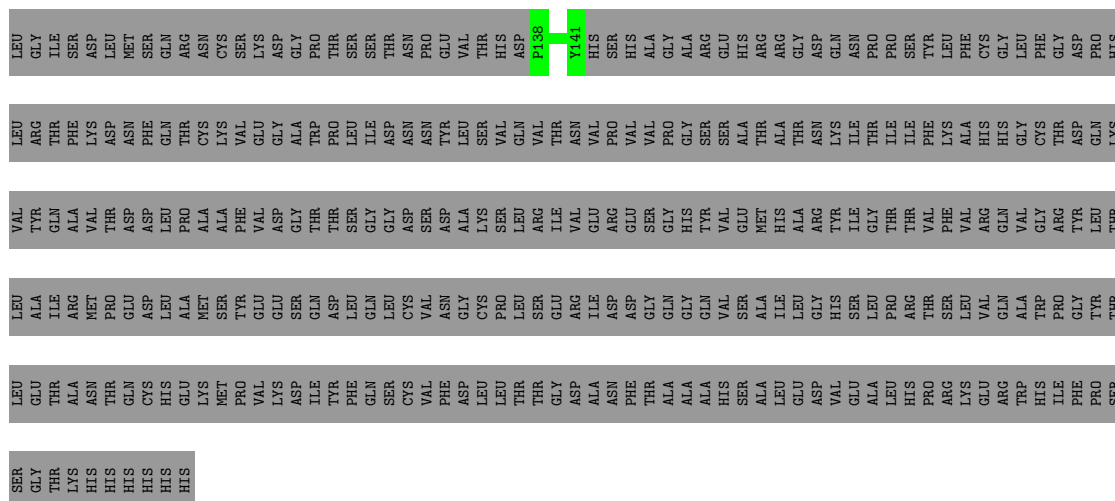
[illegible]

Chain W: .

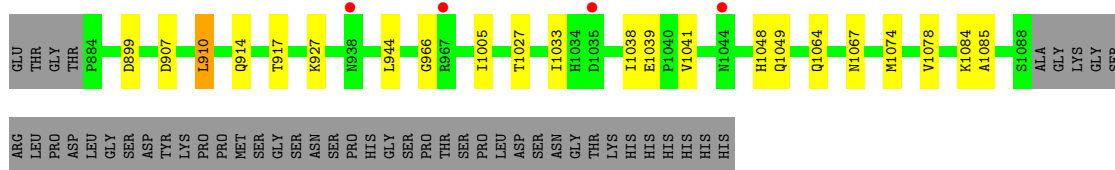
99%

Position	Most Conserved AA
1	GLU
2	THR
3	GLY
4	THR
5	GLN
6	GLN
7	GLN
8	GLN
9	GLN
10	GLN
11	GLN
12	GLN
13	GLN
14	GLN
15	GLN
16	GLN
17	GLN
18	GLN
19	GLN
20	GLN
21	GLN
22	GLN
23	GLN
24	GLN
25	GLN
26	GLN
27	GLN
28	GLN
29	GLN
30	GLN
31	GLN
32	GLN
33	GLN
34	GLN
35	GLN
36	GLN
37	GLN
38	GLN
39	GLN
40	GLN
41	GLN
42	GLN
43	GLN
44	GLN
45	GLN
46	GLN
47	GLN
48	GLN
49	GLN
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88	GLN
89	GLN
90	GLN
91	GLN
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93	GLN
94	GLN
95	GLN
96	GLN
97	GLN
98	GLN
99	P
100	Y

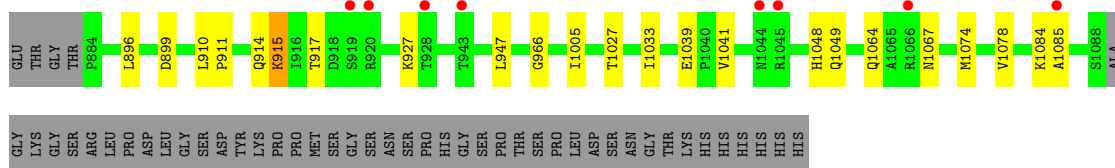
[illegible]



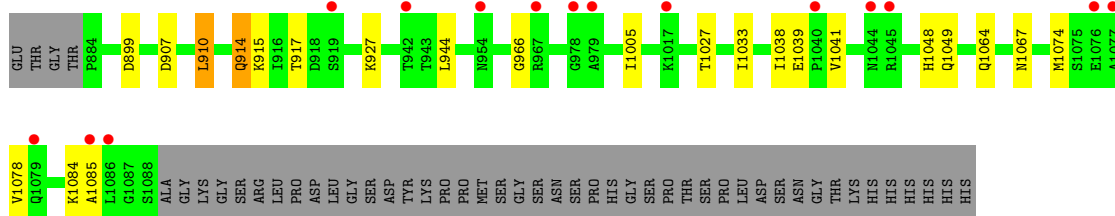
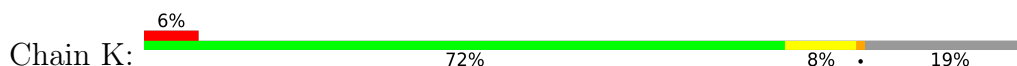
- Molecule 3: Neogenin



- Molecule 3: Neogenin

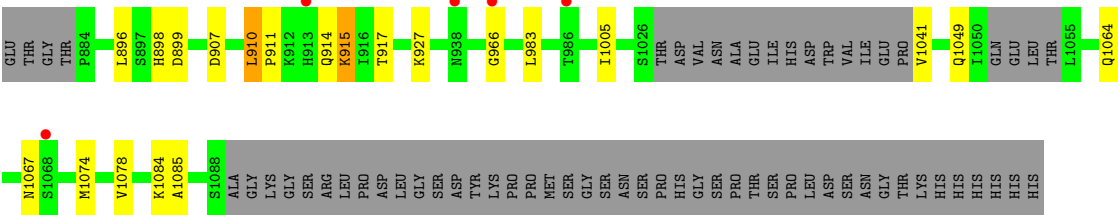


- Molecule 3: Neogenin

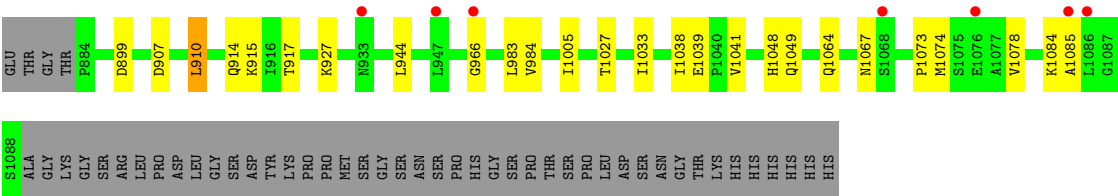


- Molecule 3: Neogenin

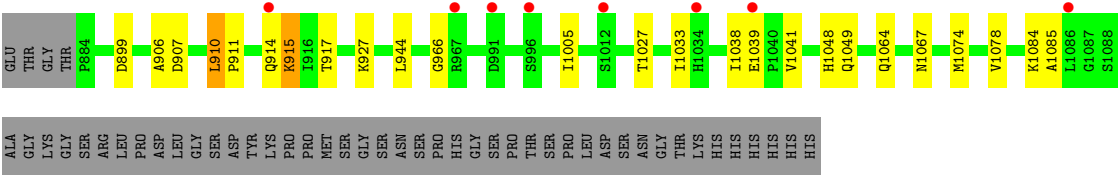




● Molecule 3: Neogenin



● Molecule 3: Neogenin



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	279.48Å 279.48Å 142.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	69.87 – 5.50 69.87 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (69.87-5.50) 99.8 (69.87-5.50)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 5.41Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, R_{free}	0.326 , 0.428 0.332 , 0.425	Depositor DCC
R_{free} test set	1062 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	193.6	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 712.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.106 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	25210	wwPDB-VP
Average B, all atoms (Å ²)	572.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.29	0/834	0.52	0/1131
1	B	0.29	0/849	0.56	0/1154
1	G	0.29	0/842	0.55	0/1143
1	H	0.29	0/832	0.52	0/1129
1	M	0.29	0/834	0.52	0/1132
1	N	0.29	0/852	0.55	0/1157
2	C	0.24	0/563	0.48	0/756
2	D	0.24	0/573	0.46	0/770
2	I	0.24	0/542	0.47	0/725
2	J	0.25	0/527	0.48	0/706
2	O	0.24	0/535	0.48	0/718
2	P	0.24	0/577	0.46	0/775
2	S	0.56	0/34	1.52	0/45
2	T	0.59	0/34	1.52	0/45
2	U	0.57	0/34	1.52	0/45
2	V	0.56	0/34	1.54	0/45
2	W	0.54	0/34	1.55	0/45
2	X	0.57	0/34	1.52	0/45
2	c	0.86	0/1243	1.26	5/1687 (0.3%)
2	d	0.86	0/1244	1.26	5/1689 (0.3%)
2	i	0.87	0/1216	1.27	4/1653 (0.2%)
2	j	0.86	0/1236	1.26	5/1679 (0.3%)
2	o	0.87	0/1232	1.26	6/1675 (0.4%)
2	p	0.86	0/1237	1.26	4/1679 (0.2%)
3	E	0.86	0/1646	1.12	4/2250 (0.2%)
3	F	0.86	0/1639	1.12	4/2240 (0.2%)
3	K	0.85	0/1647	1.12	4/2250 (0.2%)
3	L	0.86	0/1466	1.10	2/1999 (0.1%)
3	Q	0.86	0/1646	1.12	4/2248 (0.2%)
3	R	0.85	0/1639	1.12	4/2242 (0.2%)
All	All	0.72	0/25655	1.02	51/34857 (0.1%)

There are no bond length outliers.

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	o	228	ASP	N-CA-C	-6.70	100.88	110.59
2	d	228	ASP	N-CA-C	-6.66	100.93	110.59
2	j	228	ASP	N-CA-C	-6.66	100.94	110.59
2	i	228	ASP	N-CA-C	-6.64	100.96	110.59
2	p	228	ASP	N-CA-C	-6.64	100.97	110.59

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	813	0	754	14	0
1	B	828	0	785	7	0
1	G	821	0	770	9	0
1	H	811	0	752	4	0
1	M	813	0	756	3	0
1	N	831	0	789	8	0
2	C	556	0	531	5	0
2	D	566	0	546	6	0
2	I	536	0	519	4	0
2	J	522	0	479	4	0
2	O	529	0	499	3	0
2	P	570	0	549	3	0
2	S	33	0	26	0	0
2	T	33	0	26	0	0
2	U	33	0	26	0	0
2	V	33	0	26	0	0
2	W	33	0	26	0	0
2	X	33	0	26	0	0
2	c	1218	0	1178	15	0
2	d	1219	0	1182	5	0
2	i	1193	0	1142	6	0
2	j	1211	0	1164	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	o	1207	0	1160	5	0
2	p	1212	0	1167	3	0
3	E	1602	0	1584	9	0
3	F	1596	0	1578	13	0
3	K	1604	0	1599	13	0
3	L	1429	0	1416	12	0
3	Q	1603	0	1598	13	0
3	R	1596	0	1577	13	0
4	D	14	0	13	1	0
4	E	14	0	13	0	0
4	F	14	0	13	0	0
4	I	14	0	13	1	0
4	K	14	0	13	0	0
4	L	14	0	13	0	0
4	P	14	0	13	1	0
4	Q	14	0	13	0	0
4	R	14	0	13	0	0
All	All	25210	0	24347	156	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 3.

The worst 5 of 156 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:K:914:GLN:HB3	3:K:944:LEU:HD13	1.37	1.05
3:R:910:LEU:HD23	3:R:914:GLN:C	1.97	0.90
3:Q:910:LEU:HD23	3:Q:914:GLN:C	1.98	0.87
3:L:910:LEU:HD23	3:L:914:GLN:C	1.99	0.86
3:E:914:GLN:HB3	3:E:944:LEU:HD13	1.58	0.86

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	103/117 (88%)	100 (97%)	3 (3%)	0	100	100
1	B	104/117 (89%)	101 (97%)	3 (3%)	0	100	100
1	G	104/117 (89%)	101 (97%)	3 (3%)	0	100	100
1	H	103/117 (88%)	100 (97%)	3 (3%)	0	100	100
1	M	103/117 (88%)	100 (97%)	3 (3%)	0	100	100
1	N	104/117 (89%)	101 (97%)	3 (3%)	0	100	100
2	C	72/371 (19%)	72 (100%)	0	0	100	100
2	D	73/371 (20%)	72 (99%)	1 (1%)	0	100	100
2	I	67/371 (18%)	66 (98%)	1 (2%)	0	100	100
2	J	71/371 (19%)	71 (100%)	0	0	100	100
2	O	67/371 (18%)	67 (100%)	0	0	100	100
2	P	74/371 (20%)	72 (97%)	2 (3%)	0	100	100
2	S	2/371 (0%)	2 (100%)	0	0	100	100
2	T	2/371 (0%)	2 (100%)	0	0	100	100
2	U	2/371 (0%)	2 (100%)	0	0	100	100
2	V	2/371 (0%)	2 (100%)	0	0	100	100
2	W	2/371 (0%)	2 (100%)	0	0	100	100
2	X	2/371 (0%)	2 (100%)	0	0	100	100
2	c	152/371 (41%)	141 (93%)	11 (7%)	0	100	100
2	d	152/371 (41%)	141 (93%)	11 (7%)	0	100	100
2	i	152/371 (41%)	141 (93%)	11 (7%)	0	100	100
2	j	152/371 (41%)	141 (93%)	11 (7%)	0	100	100
2	o	152/371 (41%)	141 (93%)	11 (7%)	0	100	100
2	p	152/371 (41%)	141 (93%)	11 (7%)	0	100	100
3	E	203/253 (80%)	192 (95%)	10 (5%)	1 (0%)	24	64
3	F	203/253 (80%)	192 (95%)	10 (5%)	1 (0%)	24	64
3	K	203/253 (80%)	192 (95%)	10 (5%)	1 (0%)	24	64
3	L	181/253 (72%)	170 (94%)	10 (6%)	1 (1%)	21	59
3	Q	203/253 (80%)	192 (95%)	10 (5%)	1 (0%)	24	64
3	R	203/253 (80%)	192 (95%)	10 (5%)	1 (0%)	24	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3165/8898 (36%)	3011 (95%)	148 (5%)	6 (0%)	43	78

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	966	GLY
3	F	966	GLY
3	K	966	GLY
3	L	966	GLY
3	Q	966	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	91/107 (85%)	90 (99%)	1 (1%)	65	75
1	B	94/107 (88%)	93 (99%)	1 (1%)	65	75
1	G	92/107 (86%)	91 (99%)	1 (1%)	65	75
1	H	90/107 (84%)	89 (99%)	1 (1%)	65	75
1	M	91/107 (85%)	90 (99%)	1 (1%)	65	75
1	N	94/107 (88%)	93 (99%)	1 (1%)	65	75
2	C	62/317 (20%)	62 (100%)	0	100	100
2	D	64/317 (20%)	63 (98%)	1 (2%)	55	69
2	I	60/317 (19%)	60 (100%)	0	100	100
2	J	55/317 (17%)	55 (100%)	0	100	100
2	O	59/317 (19%)	59 (100%)	0	100	100
2	P	64/317 (20%)	63 (98%)	1 (2%)	55	69
2	S	4/317 (1%)	4 (100%)	0	100	100
2	T	4/317 (1%)	4 (100%)	0	100	100
2	U	4/317 (1%)	4 (100%)	0	100	100
2	V	4/317 (1%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	W	4/317 (1%)	4 (100%)	0	100	100
2	X	4/317 (1%)	4 (100%)	0	100	100
2	c	135/317 (43%)	128 (95%)	7 (5%)	21	42
2	d	135/317 (43%)	128 (95%)	7 (5%)	21	42
2	i	131/317 (41%)	125 (95%)	6 (5%)	24	45
2	j	133/317 (42%)	127 (96%)	6 (4%)	24	46
2	o	133/317 (42%)	127 (96%)	6 (4%)	24	46
2	p	133/317 (42%)	126 (95%)	7 (5%)	20	41
3	E	178/222 (80%)	172 (97%)	6 (3%)	32	54
3	F	177/222 (80%)	172 (97%)	5 (3%)	38	59
3	K	179/222 (81%)	172 (96%)	7 (4%)	28	49
3	L	156/222 (70%)	150 (96%)	6 (4%)	29	50
3	Q	179/222 (81%)	172 (96%)	7 (4%)	28	49
3	R	177/222 (80%)	170 (96%)	7 (4%)	28	49
All	All	2786/7680 (36%)	2701 (97%)	85 (3%)	35	56

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	d	260	ILE
2	j	269	VAL
2	d	269	VAL
2	i	269	VAL
2	o	260	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	d	214	ASN
2	i	214	ASN
2	p	223	HIS
2	o	214	ASN
2	p	214	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	$\# Z > 2$
4	NAG	I	1001	2	14,14,15	0.47	0	17,19,21	0.66	0
4	NAG	F	2001	3	14,14,15	0.34	0	17,19,21	0.72	1 (5%)
4	NAG	E	2001	3	14,14,15	0.33	0	17,19,21	0.73	1 (5%)
4	NAG	R	2001	3	14,14,15	0.30	0	17,19,21	0.72	1 (5%)
4	NAG	P	1001	2	14,14,15	0.48	0	17,19,21	0.67	0
4	NAG	D	1001	2	14,14,15	0.44	0	17,19,21	0.65	0
4	NAG	Q	2001	3	14,14,15	0.29	0	17,19,21	0.76	1 (5%)
4	NAG	K	2001	3	14,14,15	0.32	0	17,19,21	0.74	1 (5%)
4	NAG	L	2001	3	14,14,15	0.29	0	17,19,21	0.75	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
4	NAG	I	1001	2	-	0/6/23/26	0/1/1/1
4	NAG	F	2001	3	-	0/6/23/26	0/1/1/1
4	NAG	E	2001	3	-	0/6/23/26	0/1/1/1
4	NAG	R	2001	3	-	0/6/23/26	0/1/1/1
4	NAG	P	1001	2	-	0/6/23/26	0/1/1/1
4	NAG	D	1001	2	-	0/6/23/26	0/1/1/1
4	NAG	Q	2001	3	-	0/6/23/26	0/1/1/1
4	NAG	K	2001	3	-	0/6/23/26	0/1/1/1
4	NAG	L	2001	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	2001	NAG	C1-O5-C5	2.86	116.02	112.19
4	L	2001	NAG	C1-O5-C5	2.79	115.92	112.19
4	K	2001	NAG	C1-O5-C5	2.75	115.87	112.19
4	F	2001	NAG	C1-O5-C5	2.70	115.80	112.19
4	E	2001	NAG	C1-O5-C5	2.69	115.78	112.19

There are no chirality outliers.

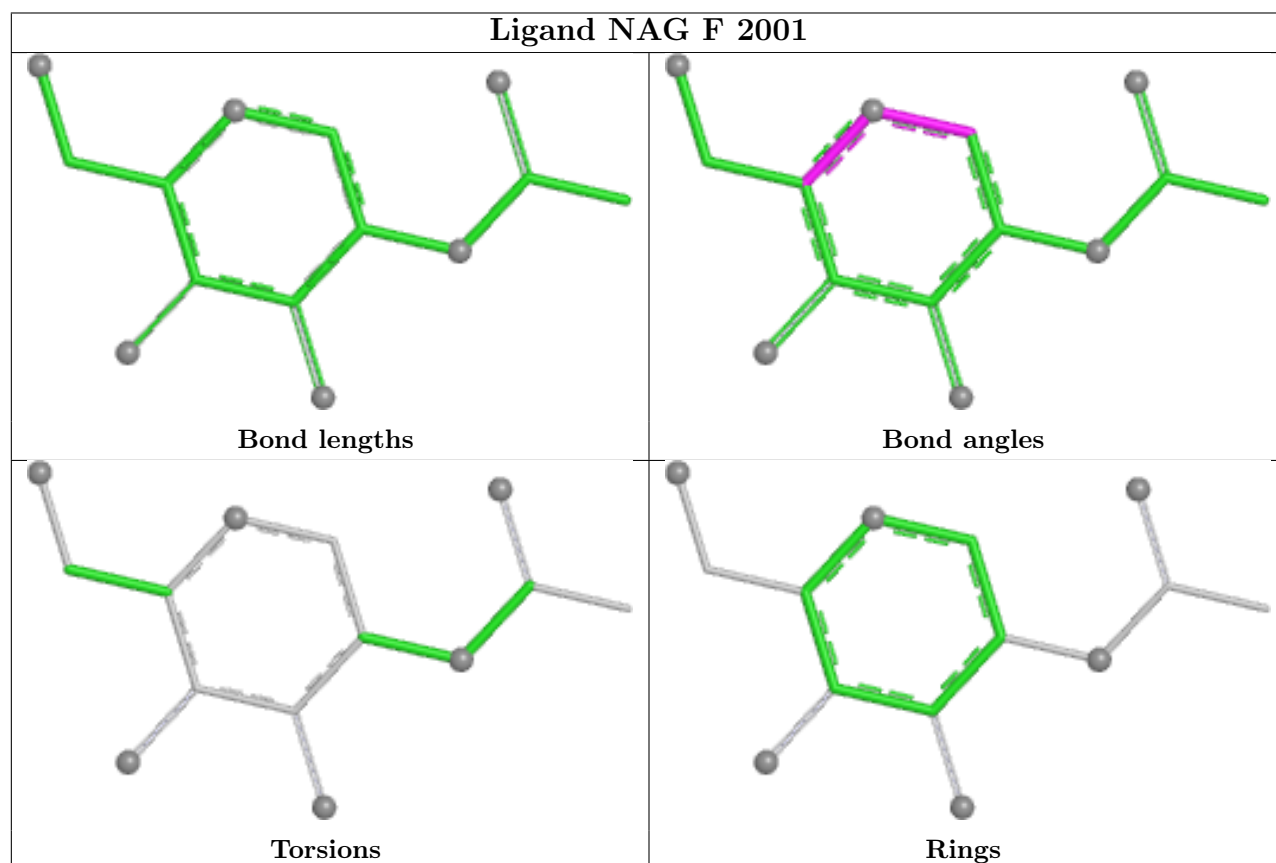
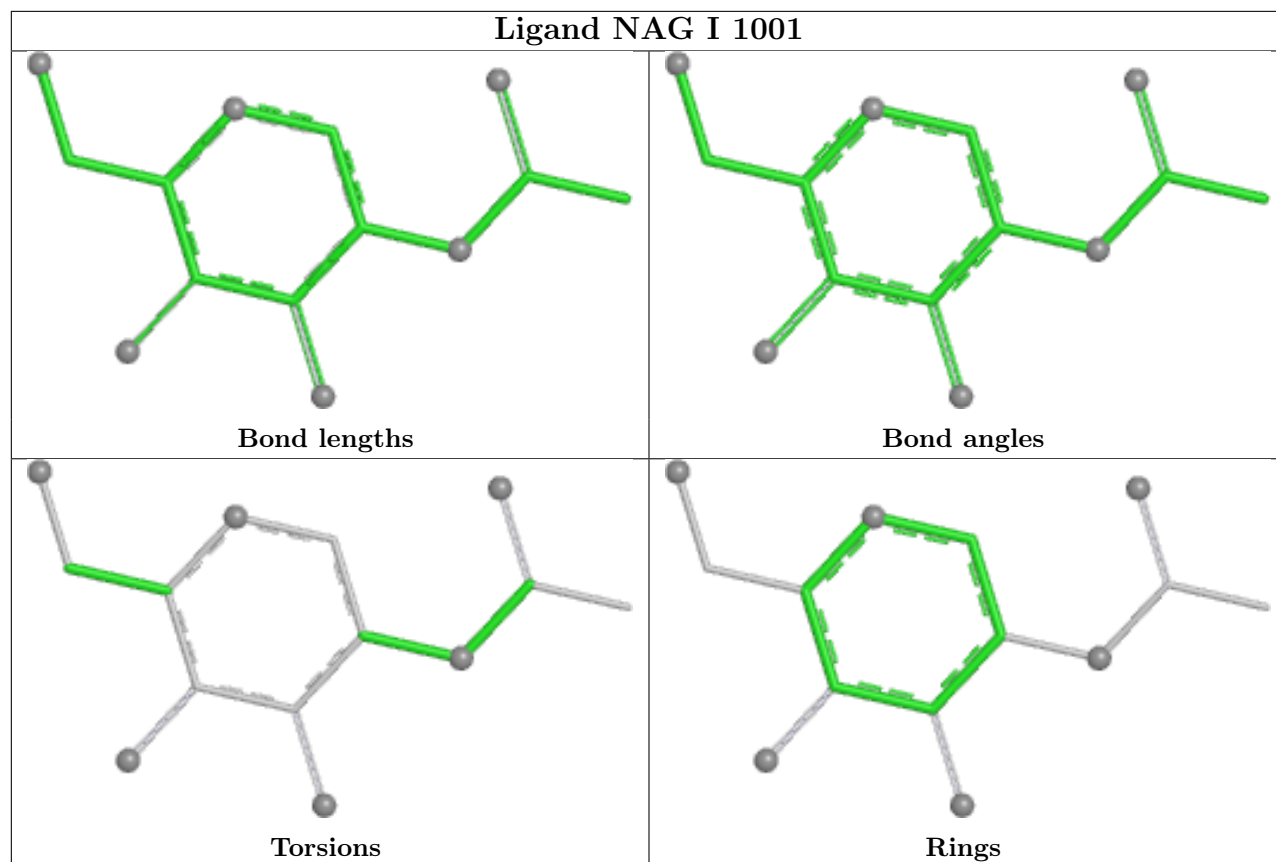
There are no torsion outliers.

There are no ring outliers.

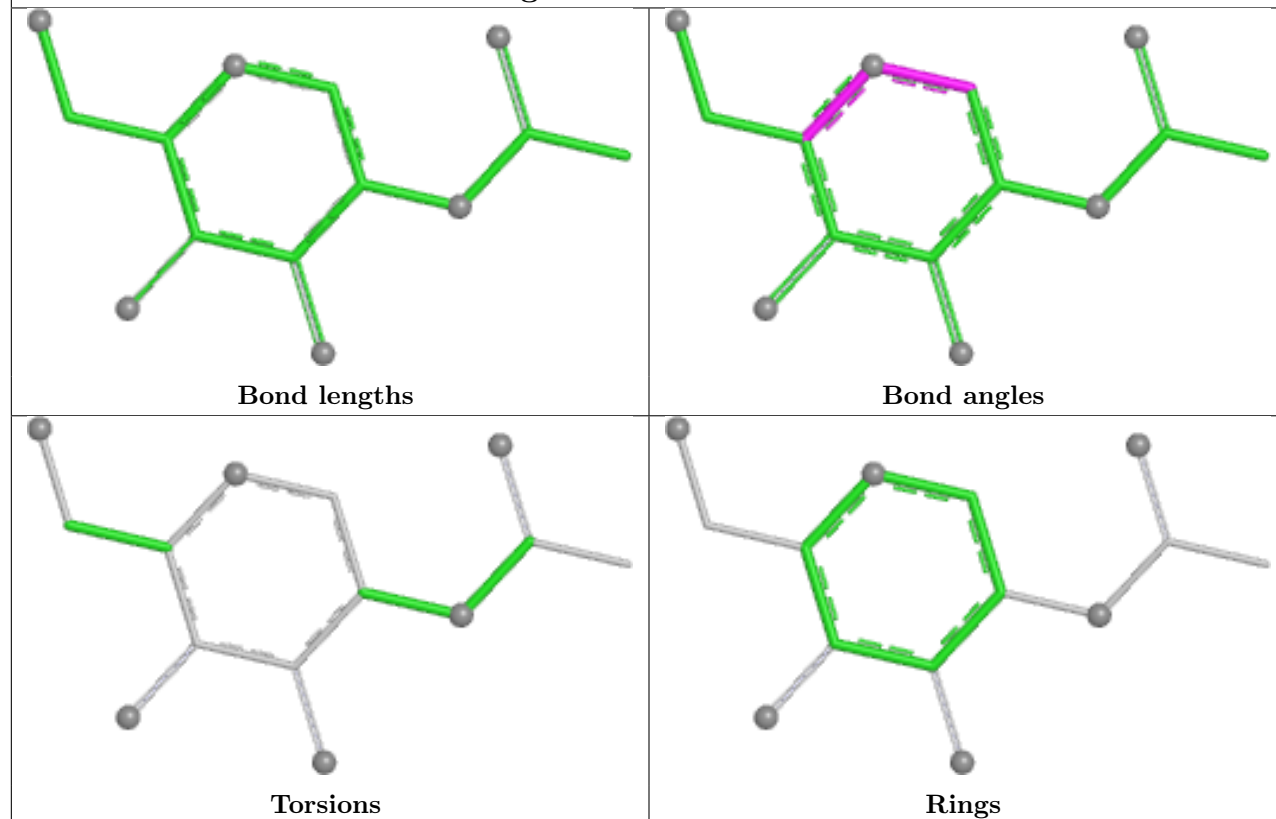
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1001	NAG	1	0
4	P	1001	NAG	1	0
4	D	1001	NAG	1	0

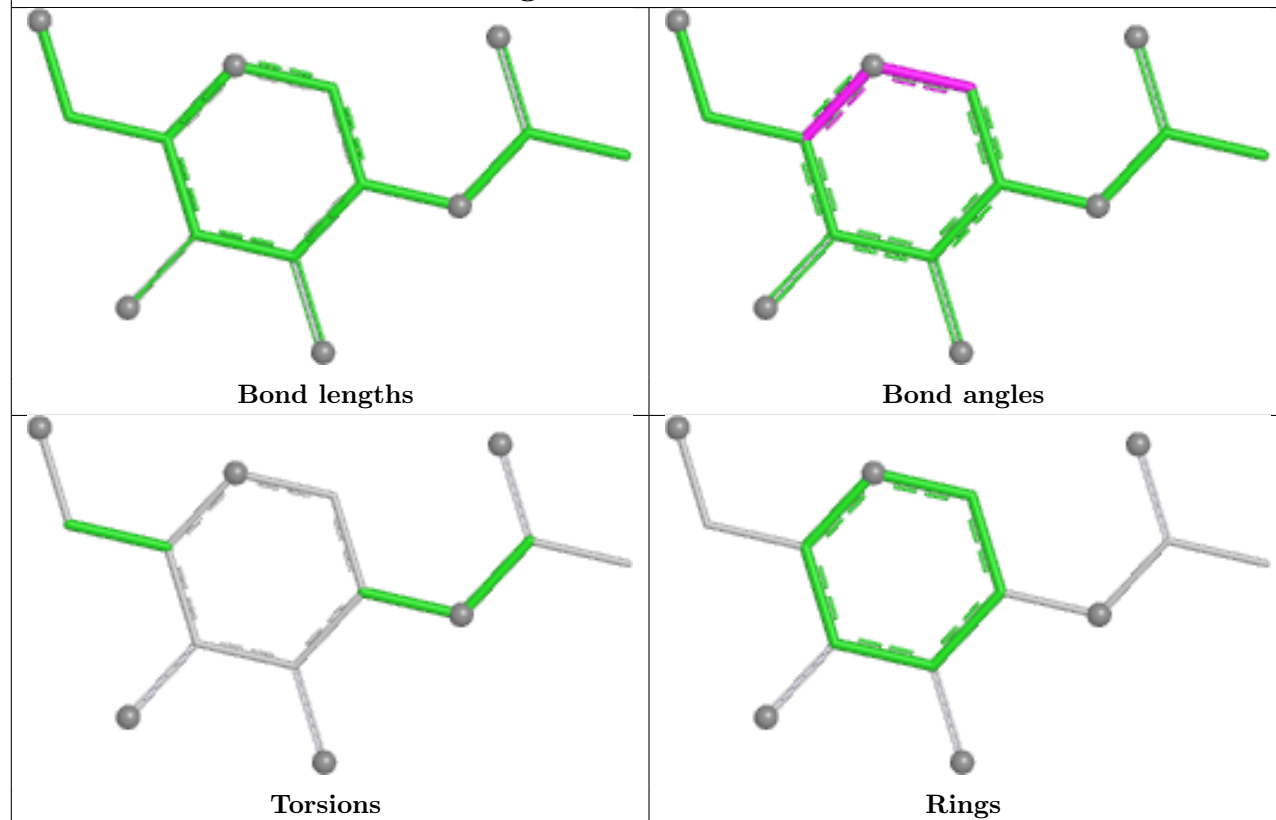
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



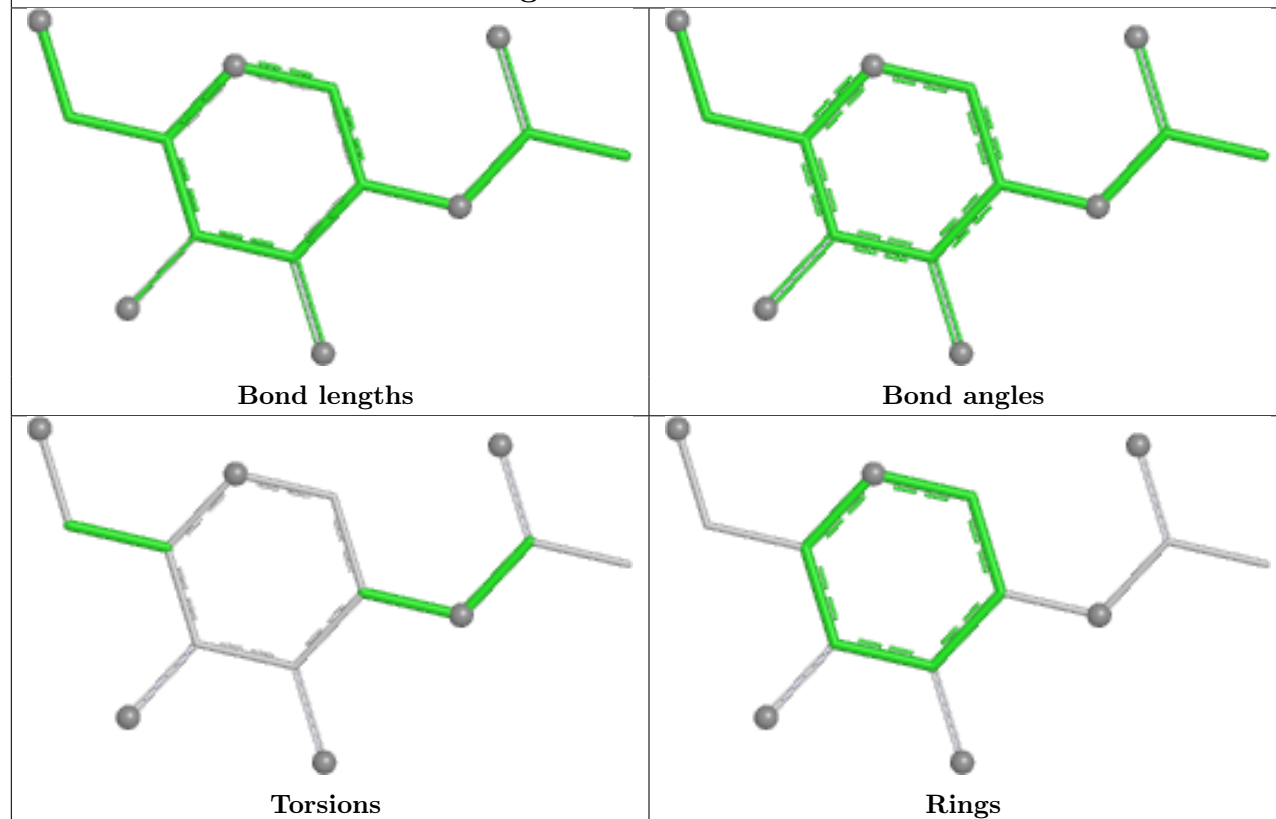
Ligand NAG E 2001



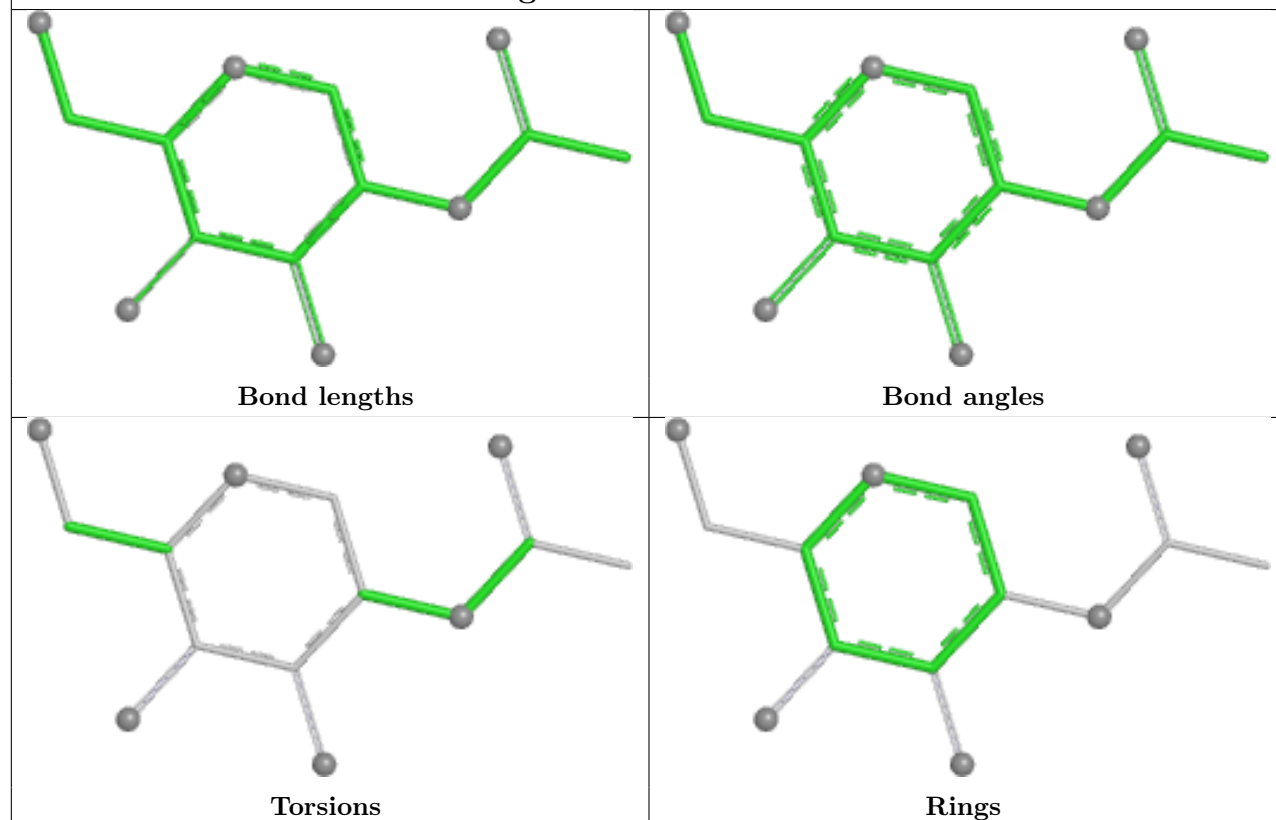
Ligand NAG R 2001



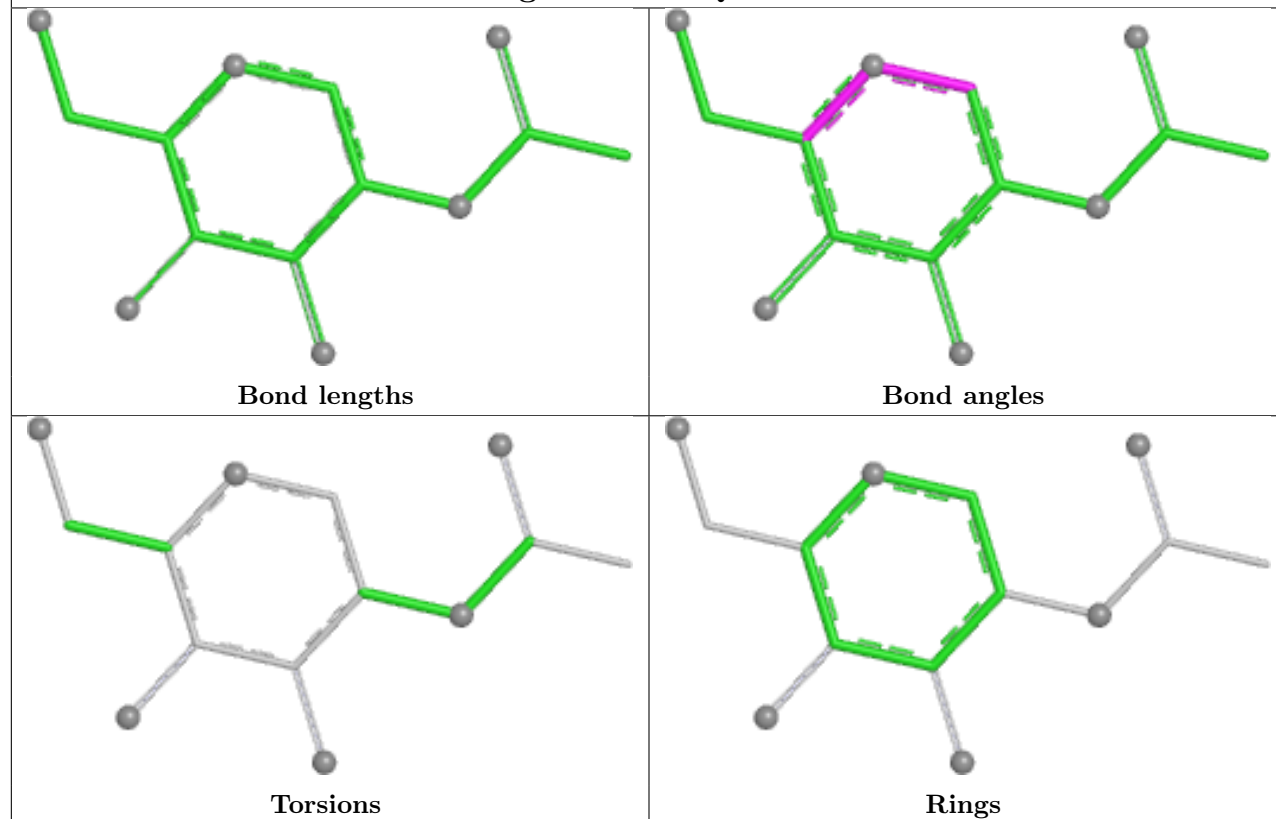
Ligand NAG P 1001



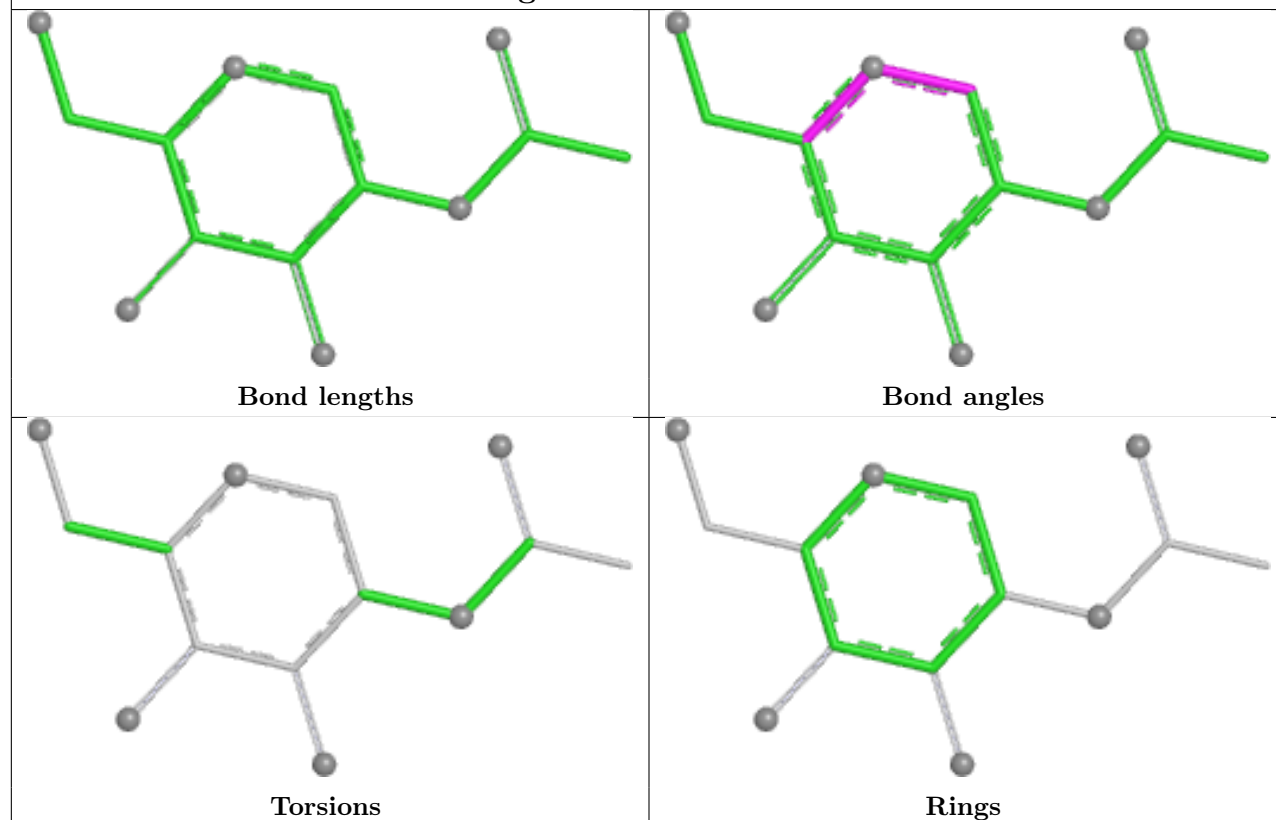
Ligand NAG D 1001

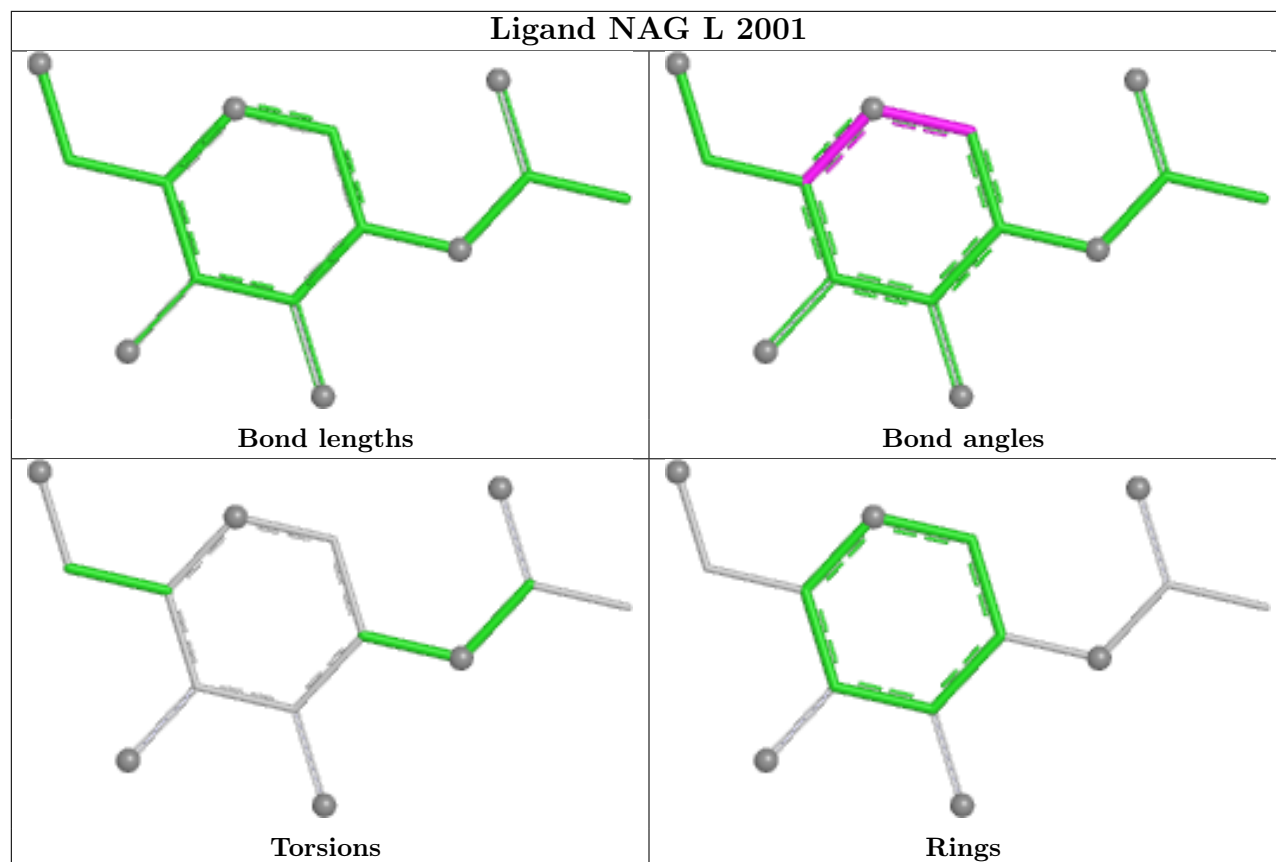


Ligand NAG Q 2001



Ligand NAG K 2001





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	105/117 (89%)	0.34	3 (2%) 53 46	263, 487, 834, 1123	0
1	B	106/117 (90%)	0.31	5 (4%) 36 36	294, 448, 732, 1355	0
1	G	106/117 (90%)	0.40	4 (3%) 44 41	497, 668, 1144, 1418	0
1	H	105/117 (89%)	0.52	4 (3%) 44 41	409, 610, 1238, 1382	0
1	M	105/117 (89%)	0.23	2 (1%) 66 55	291, 437, 645, 833	0
1	N	106/117 (90%)	0.26	2 (1%) 66 55	331, 475, 714, 889	0
2	C	74/371 (19%)	0.47	3 (4%) 41 39	445, 635, 1070, 1345	0
2	D	75/371 (20%)	0.55	2 (2%) 56 47	437, 601, 973, 1267	0
2	I	71/371 (19%)	0.88	10 (14%) 6 13	395, 608, 923, 1126	0
2	J	73/371 (19%)	0.40	7 (9%) 13 20	475, 655, 1059, 1377	0
2	O	71/371 (19%)	0.61	5 (7%) 22 27	336, 563, 942, 1080	0
2	P	76/371 (20%)	0.43	7 (9%) 14 20	321, 506, 837, 1111	0
2	S	4/371 (1%)	0.19	0 100 100	473, 552, 694, 765	0
2	T	4/371 (1%)	0.43	0 100 100	367, 402, 403, 446	0
2	U	4/371 (1%)	0.25	0 100 100	520, 598, 634, 634	0
2	V	4/371 (1%)	1.42	2 (50%) 0 3	647, 672, 704, 1135	0
2	W	4/371 (1%)	1.31	2 (50%) 0 3	454, 592, 620, 692	0
2	X	4/371 (1%)	0.62	0 100 100	523, 547, 698, 741	0
2	c	158/371 (42%)	0.32	3 (1%) 66 55	345, 469, 707, 1046	0
2	d	158/371 (42%)	0.38	8 (5%) 33 34	236, 418, 637, 1075	0
2	i	158/371 (42%)	0.47	12 (7%) 20 25	411, 606, 1038, 1142	0
2	j	158/371 (42%)	0.65	11 (6%) 22 27	530, 675, 1149, 1423	0
2	o	158/371 (42%)	0.27	6 (3%) 44 41	283, 465, 686, 941	0
2	p	158/371 (42%)	0.20	6 (3%) 44 41	447, 541, 885, 1151	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	E	205/253 (81%)	0.20	4 (1%) 65 54	227, 441, 728, 880	0
3	F	205/253 (81%)	0.17	8 (3%) 43 40	203, 391, 582, 920	0
3	K	205/253 (81%)	0.43	15 (7%) 21 25	461, 635, 1012, 1348	0
3	L	187/253 (73%)	0.26	5 (2%) 56 47	511, 642, 1112, 1460	0
3	Q	205/253 (81%)	0.12	7 (3%) 48 43	204, 422, 604, 785	0
3	R	205/253 (81%)	0.37	8 (3%) 43 40	430, 569, 836, 1135	0
All	All	3257/8898 (36%)	0.35	151 (4%) 37 36	203, 543, 962, 1460	0

The worst 5 of 151 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	p	222	ALA	5.8
1	A	501	ARG	5.0
2	O	80	GLU	4.9
2	d	222	ALA	4.9
3	K	1086	LEU	4.8

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	K	2001	14/15	0.85	0.11	447,447,447,447	0
4	NAG	P	1001	14/15	0.85	0.13	572,595,615,616	0
4	NAG	I	1001	14/15	0.91	0.09	677,688,699,706	0
4	NAG	L	2001	14/15	0.92	0.18	447,447,447,447	0

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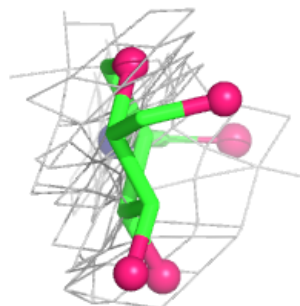
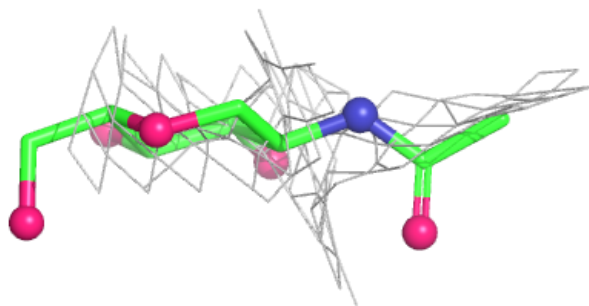
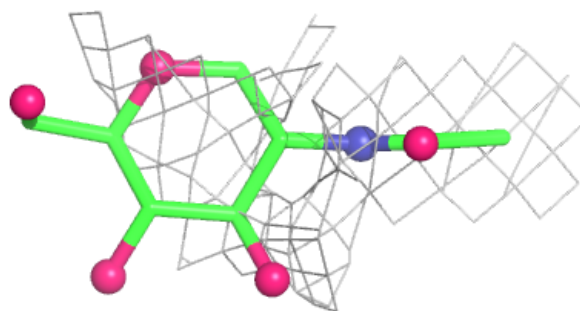
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	R	2001	14/15	0.92	0.16	447,447,447,447	0
4	NAG	Q	2001	14/15	0.95	0.15	447,447,447,447	0
4	NAG	D	1001	14/15	0.96	0.08	696,718,742,755	0
4	NAG	E	2001	14/15	0.96	0.13	447,447,447,447	0
4	NAG	F	2001	14/15	0.97	0.12	447,447,447,447	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.

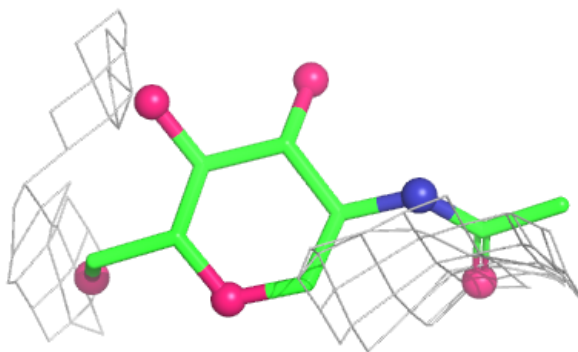
Electron density around NAG K 2001:

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

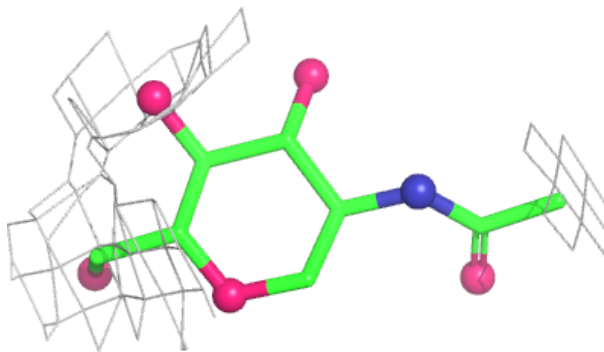


Electron density around NAG P 1001:

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

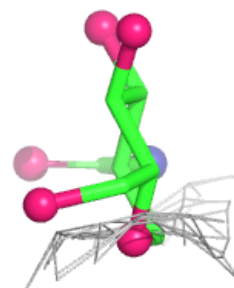
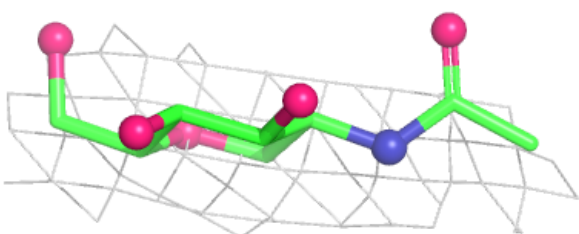
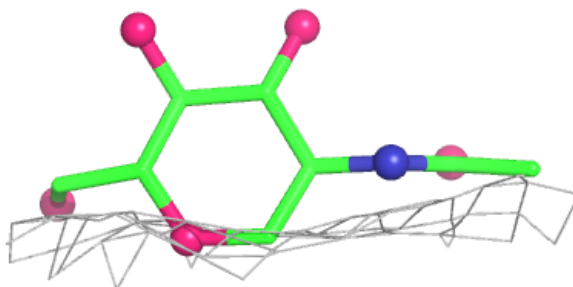
**Electron density around NAG I 1001:**

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

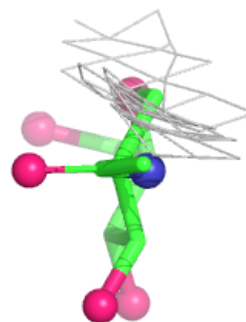
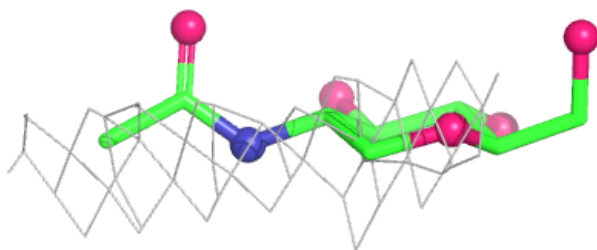
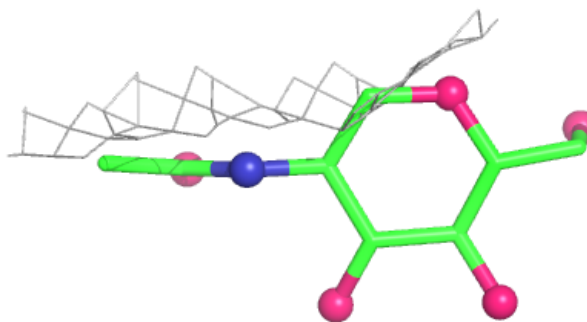


Electron density around NAG L 2001:

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

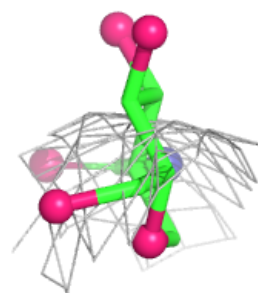
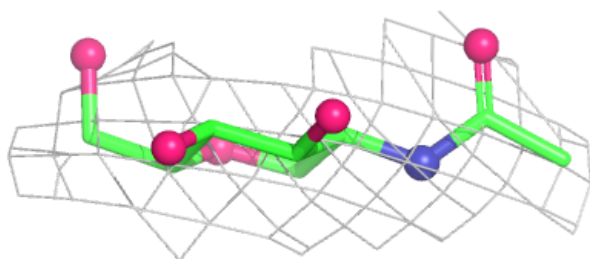
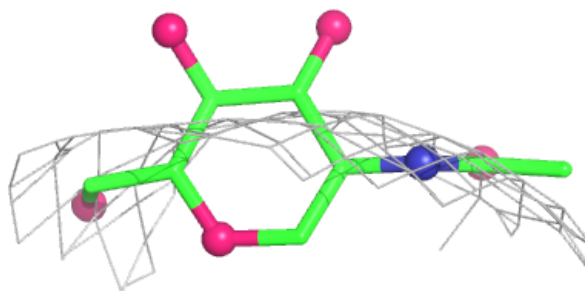
**Electron density around NAG R 2001:**

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

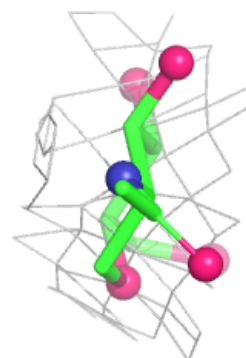
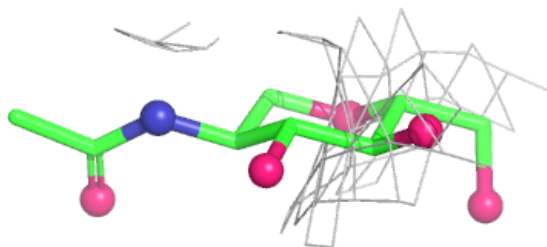
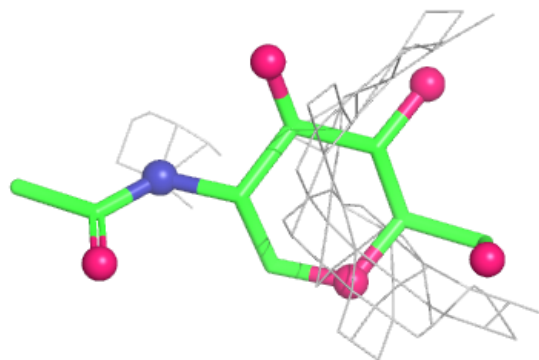


Electron density around NAG Q 2001:

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

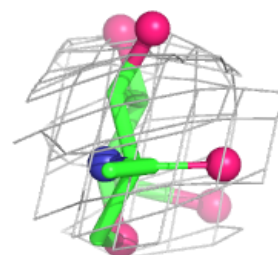
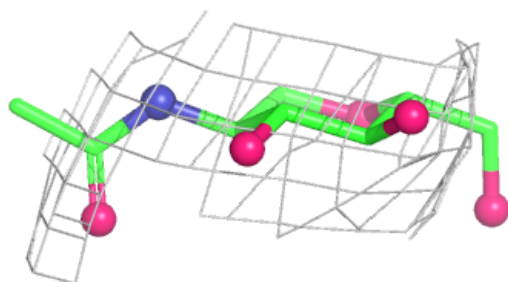
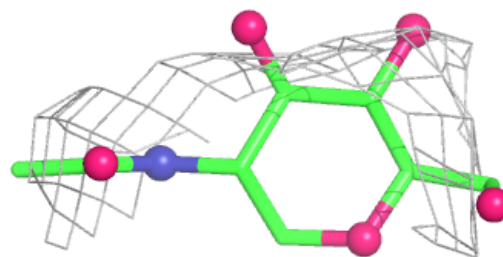
**Electron density around NAG D 1001:**

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

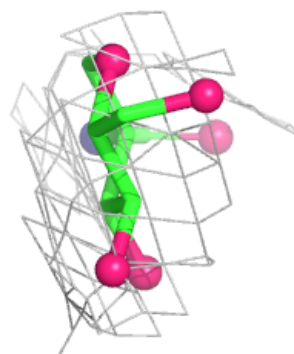
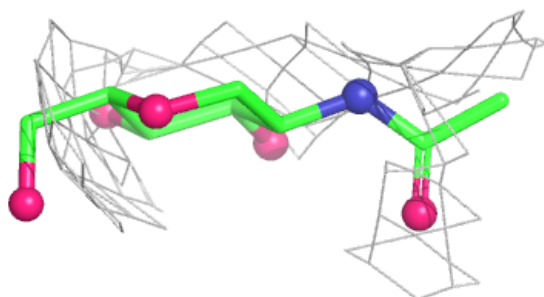
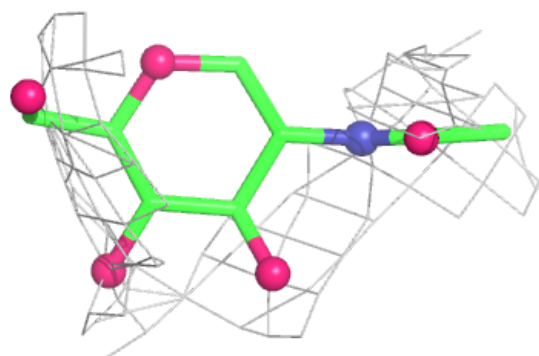


Electron density around NAG E 2001:

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

**Electron density around NAG F 2001:**

$2mF_o-DF_c$ (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.