Full wwPDB X-ray Structure Validation Report ⓘ

Jul 20, 2023 – 01:29 pm BST

PDB ID	:	6Z3M
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 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:

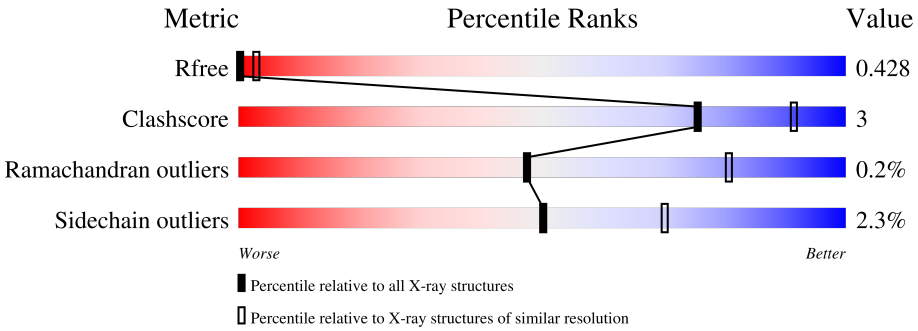
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 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}	130704	1019 (7.12-3.82)
Clashscore	141614	1010 (7.10-3.90)
Ramachandran outliers	138981	1014 (7.12-3.82)
Sidechain outliers	138945	1191 (7.20-3.80)

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%

Mol	Chain	Length	Quality of chain
1	A	117	85% • • 10%
1	B	117	85% 5% • 9%
1	G	117	85% 5% • 9%
1	H	117	85% • • 10%
1	M	117	85% • • 10%
1	N	117	85% • • 9%
2	C	371	18% • 80%

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Mol	Chain	Length	Quality of chain
2	D	371	18% 80%
2	I	371	18% 81%
2	J	371	18% 80%
2	O	371	18% 81%
2	P	371	19% 80%
2	S	371	99%
2	T	371	99%
2	U	371	99%
2	V	371	99%
2	W	371	99%
2	X	371	99%
2	c	371	41% 57%
2	d	371	41% 57%
2	i	371	41% 57%
2	j	371	41% 57%
2	o	371	41% 57%
2	p	371	41% 57%
3	E	253	75% 6% 19%
3	F	253	74% 6% 19%
3	K	253	75% 6% 19%
3	L	253	67% 6% 26%
3	Q	253	73% 7% 19%
3	R	253	74% 6% 19%

2 Entry composition (i)

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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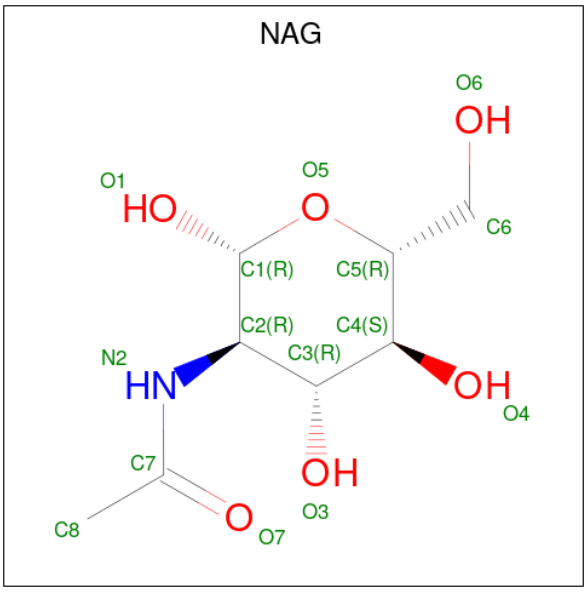
Chain	Residue	Modelled	Actual	Comment	Reference
R	882	GLY	-	expression tag	UNP P97798
R	1124	GLY	-	expression tag	UNP P97798
R	1125	THR	-	expression tag	UNP P97798
R	1126	LYS	-	expression tag	UNP P97798
R	1127	HIS	-	expression tag	UNP P97798
R	1128	HIS	-	expression tag	UNP P97798
R	1129	HIS	-	expression 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 (three-letter code: 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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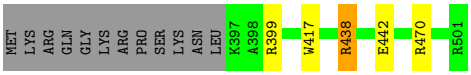
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	P	1	Total	C	N	O	0	0
			14	8	1	5		
4	Q	1	Total	C	N	O	0	0
			14	8	1	5		
4	R	1	Total	C	N	O	0	0
			14	8	1	5		

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. 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. 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.

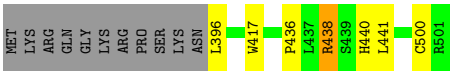
- Molecule 1: Growth/differentiation factor 5

Chain A:



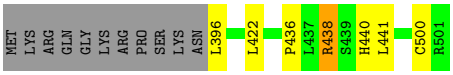
- Molecule 1: Growth/differentiation factor 5

Chain B:



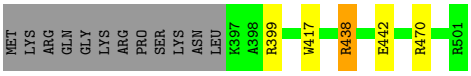
- Molecule 1: Growth/differentiation factor 5

Chain G:



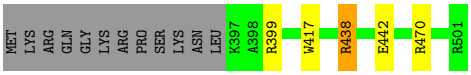
- Molecule 1: Growth/differentiation factor 5

Chain H:



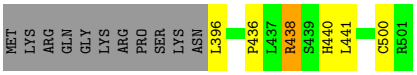
- Molecule 1: Growth/differentiation factor 5

Chain M:



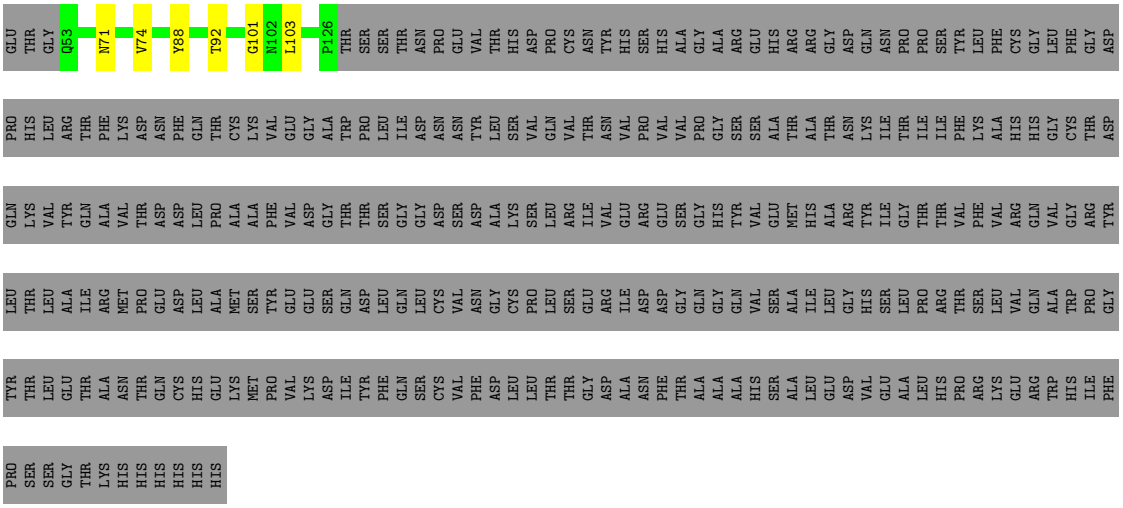
- Molecule 1: Growth/differentiation factor 5

Chain N:



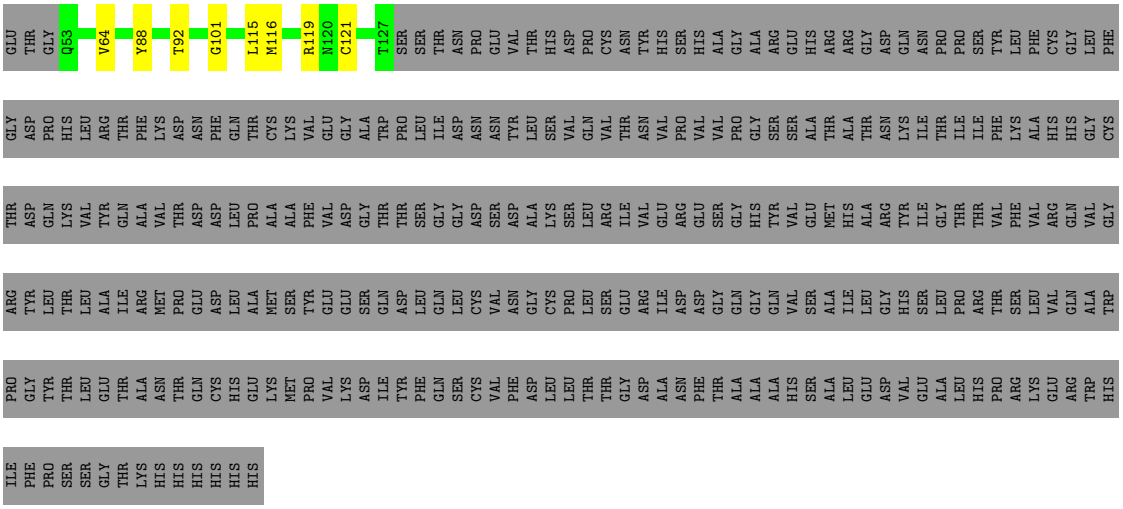
• Molecule 2: RGM domain family member B

Chain C:



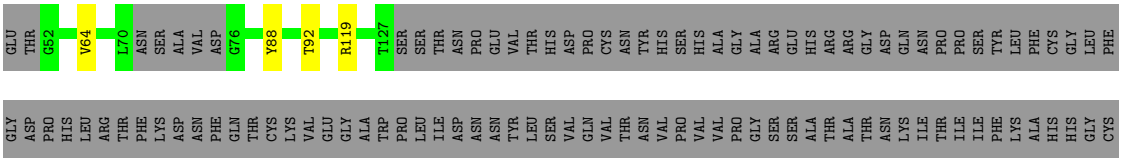
• Molecule 2: RGM domain family member B

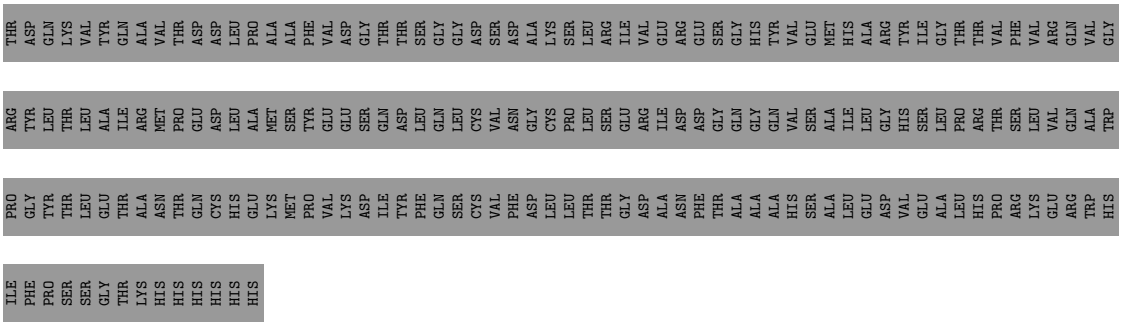
Chain D:



• Molecule 2: RGM domain family member B

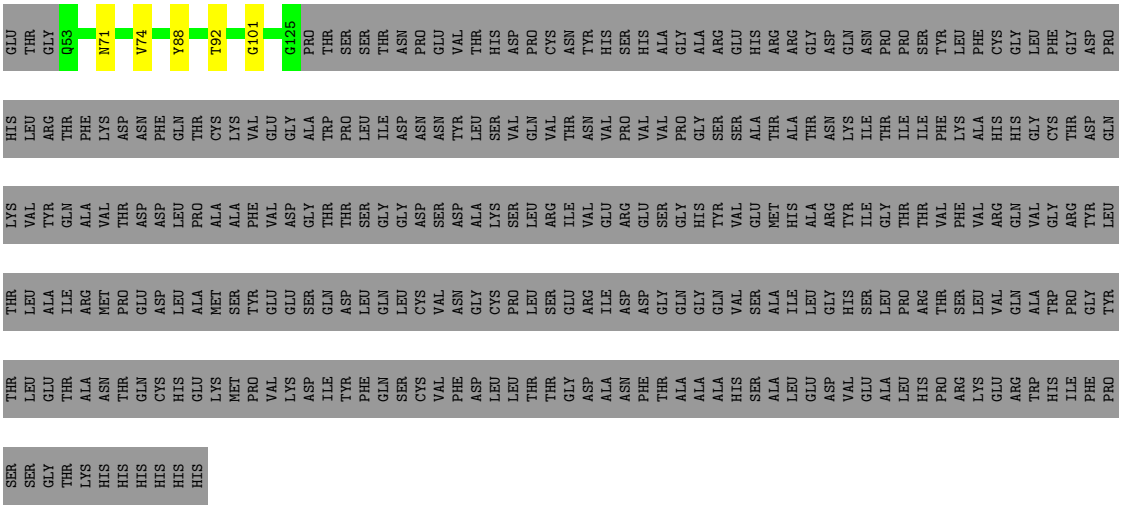
Chain I:





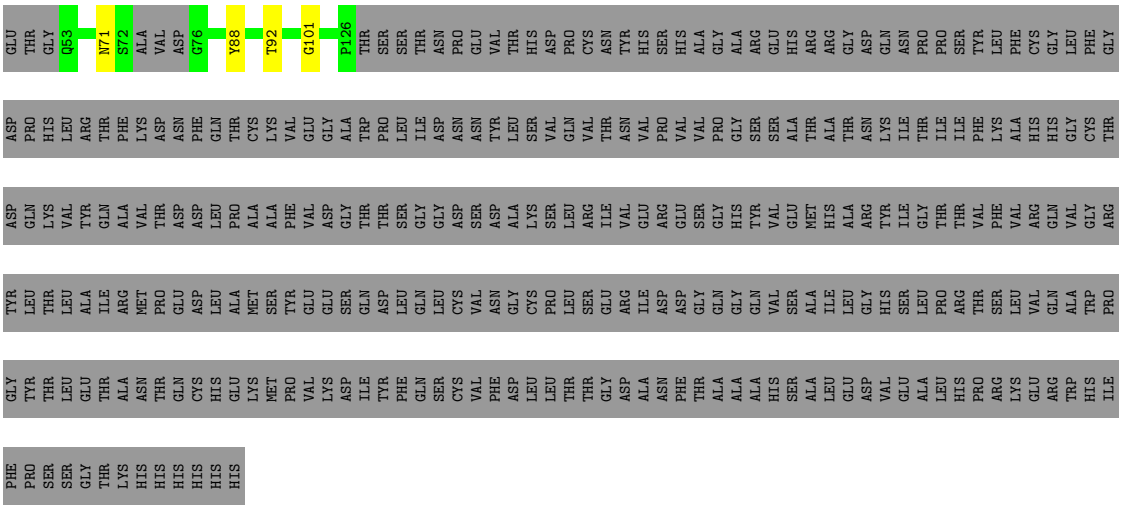
• Molecule 2: RGM domain family member B

Chain J:



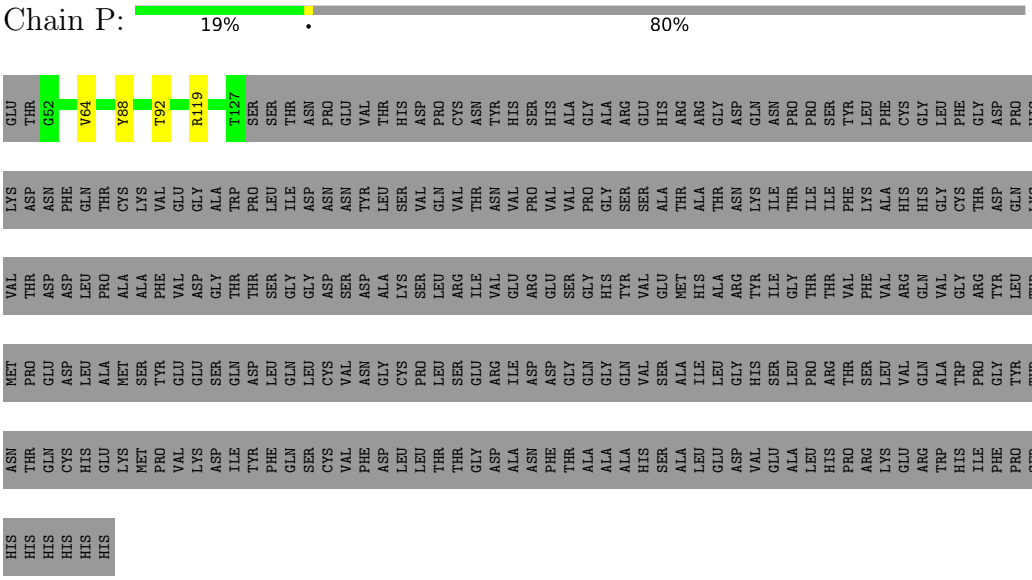
• Molecule 2: RGM domain family member B

Chain O:



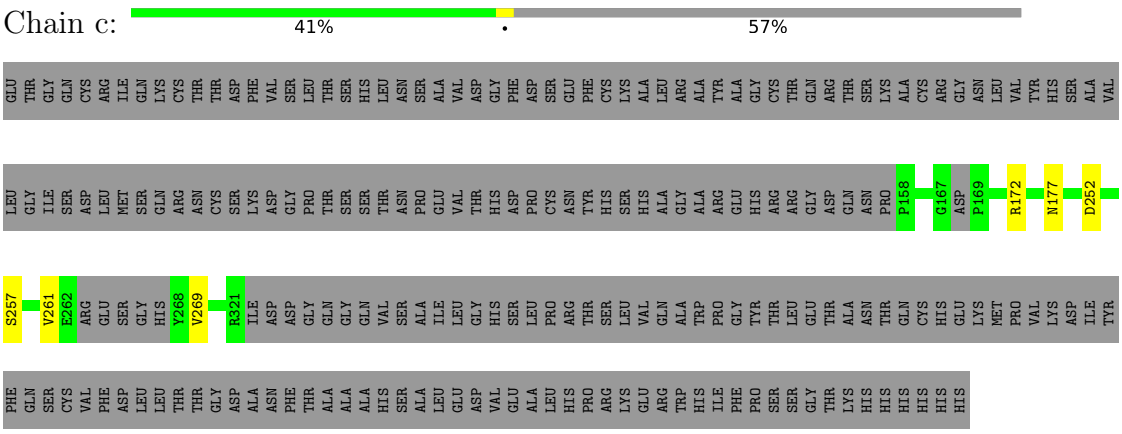
• Molecule 2: RGM domain family member B

Chain P:



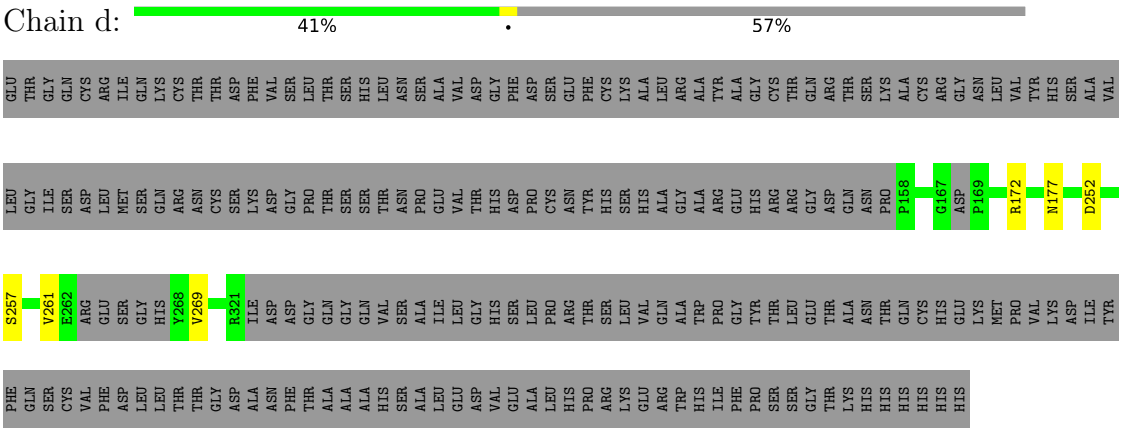
• Molecule 2: RGM domain family member B

Chain c:



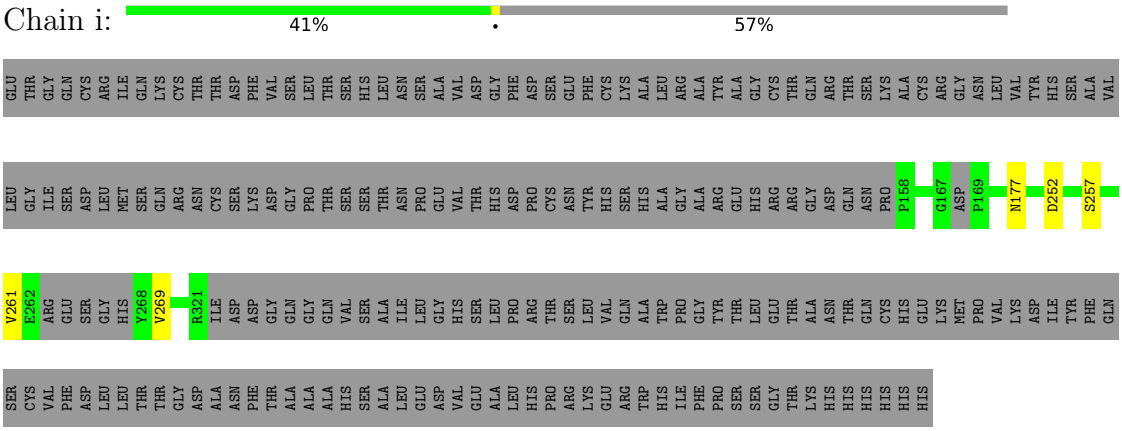
• Molecule 2: RGM domain family member B

Chain d:



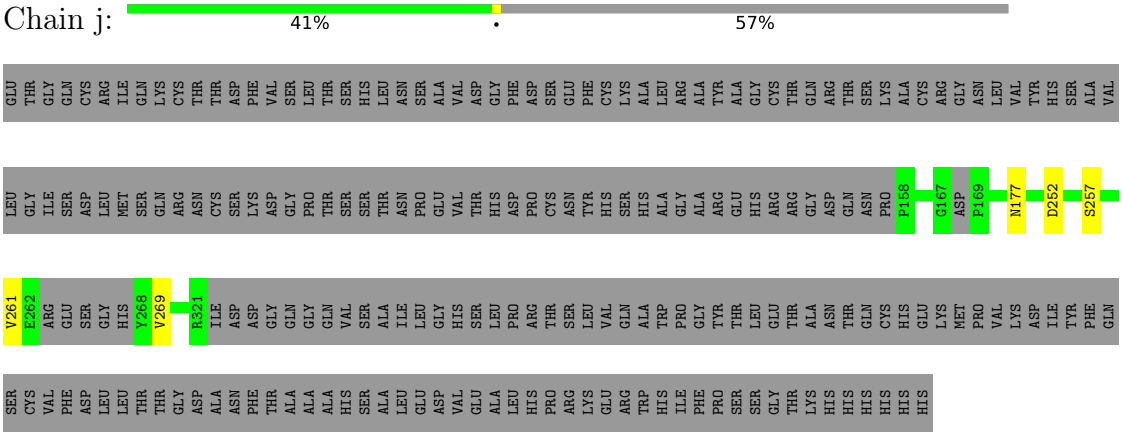
• Molecule 2: RGM domain family member B

Chain i:



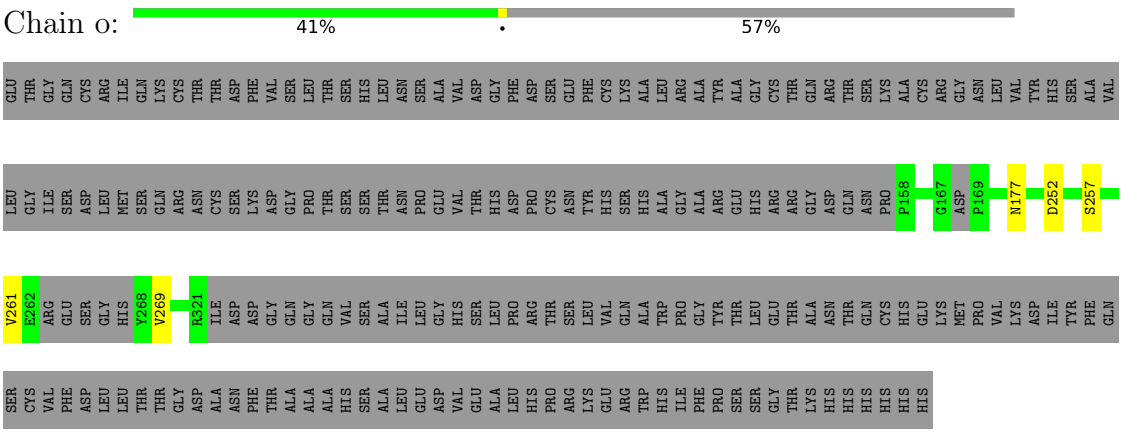
• Molecule 2: RGM domain family member B

Chain j:



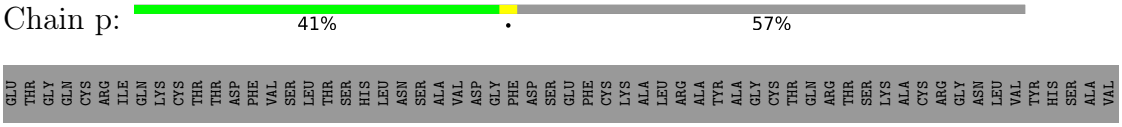
• Molecule 2: RGM domain family member B

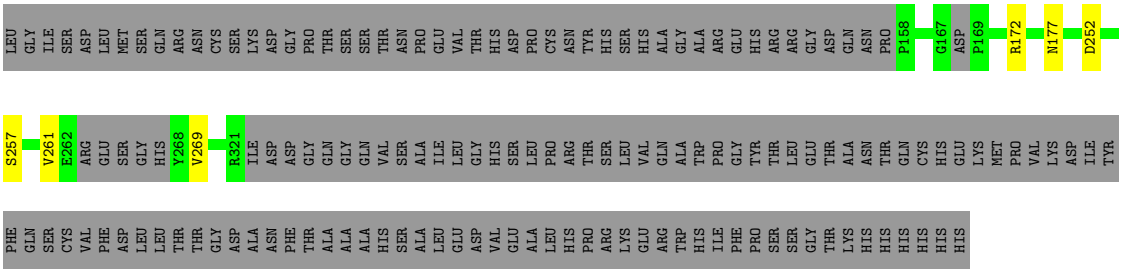
Chain o:



• Molecule 2: RGM domain family member B

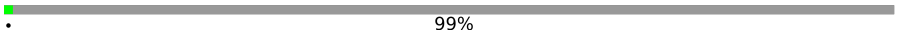
Chain p:

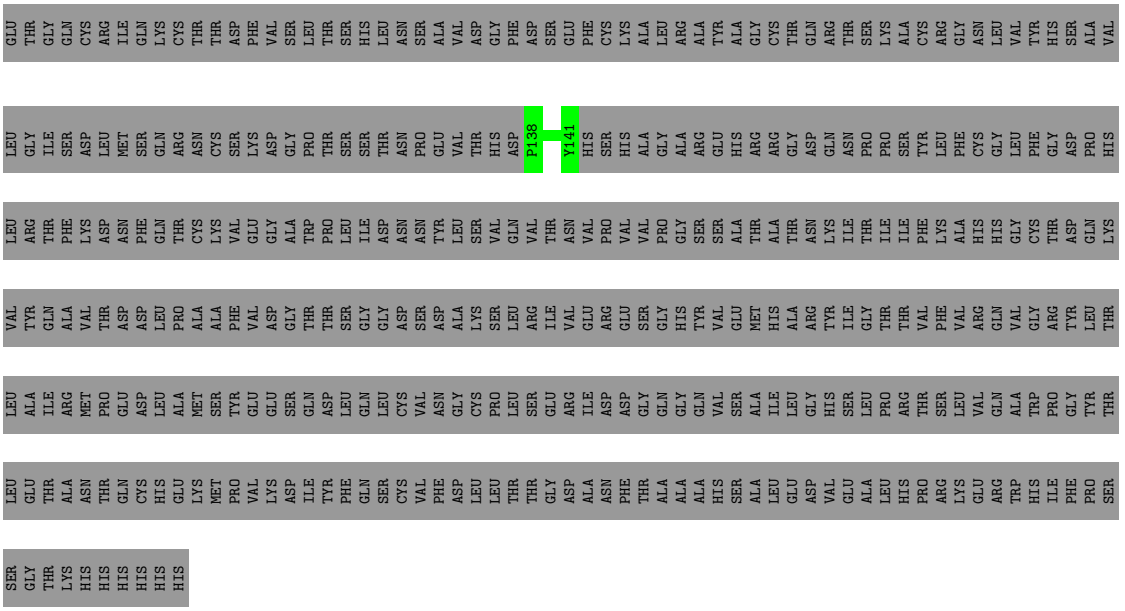




• Molecule 2: RGM domain family member B

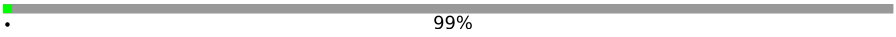
Chain S:

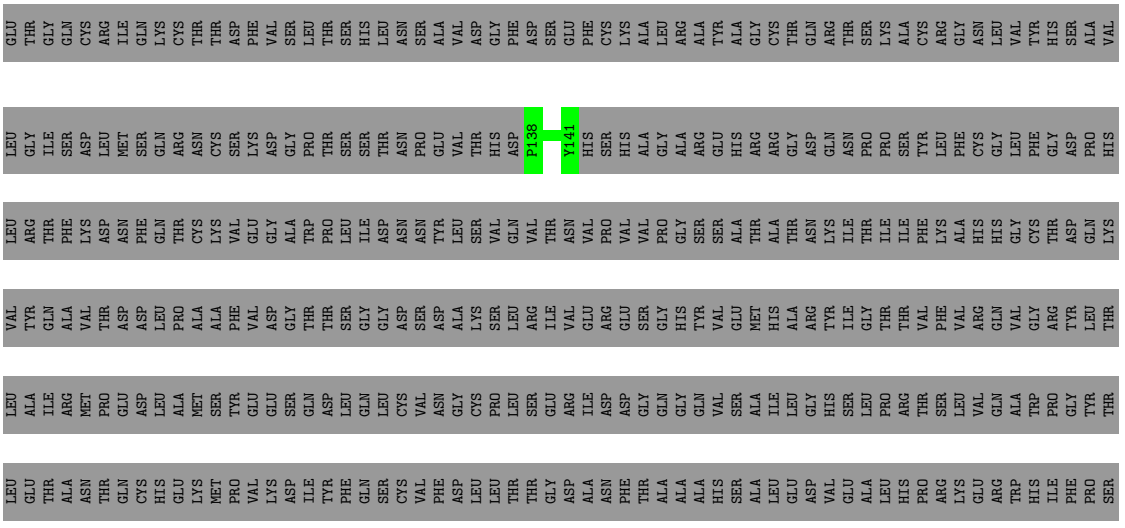




• Molecule 2: RGM domain family member B

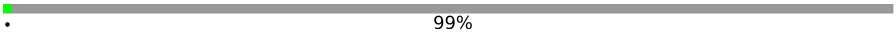
Chain T:

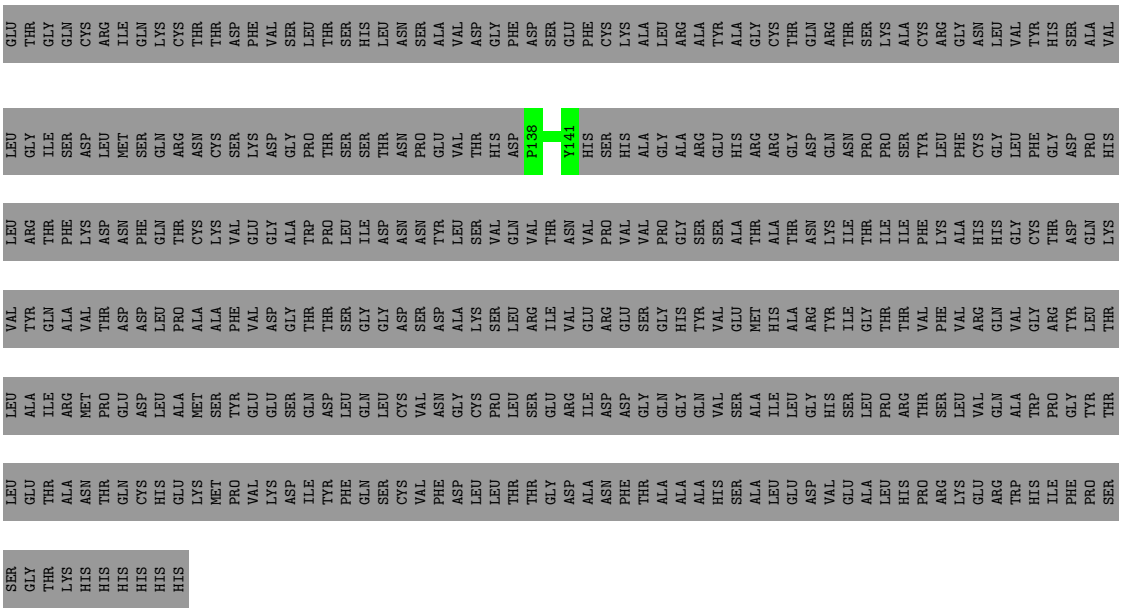




• Molecule 2: RGM domain family member B

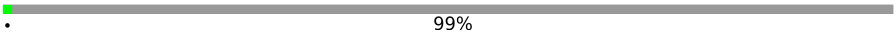
Chain U:

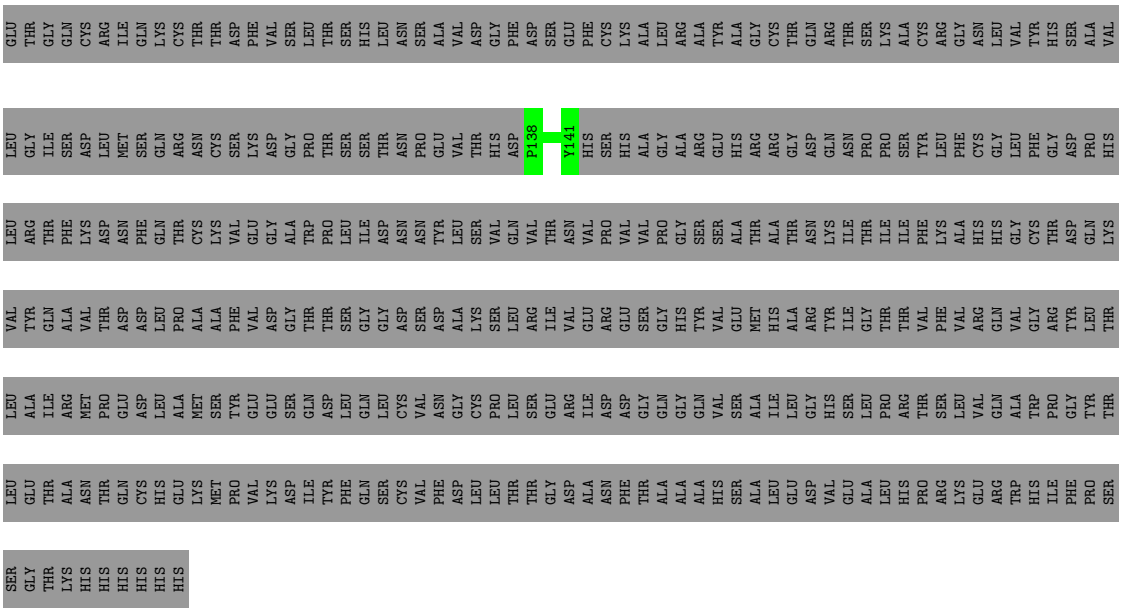




• Molecule 2: RGM domain family member B

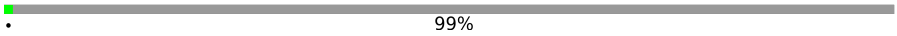
Chain V:

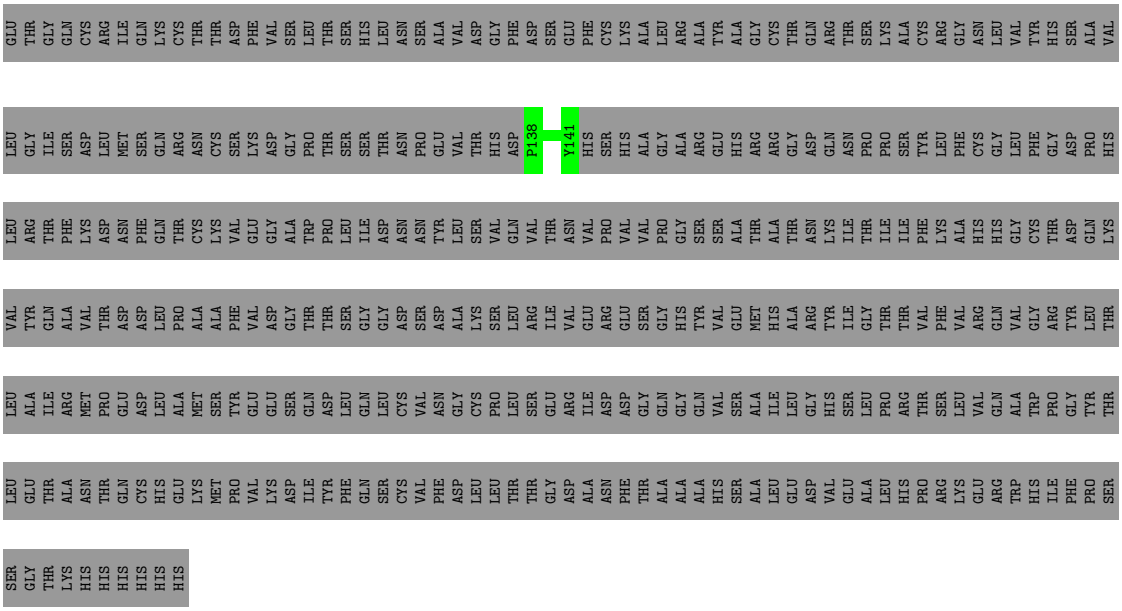




• Molecule 2: RGM domain family member B

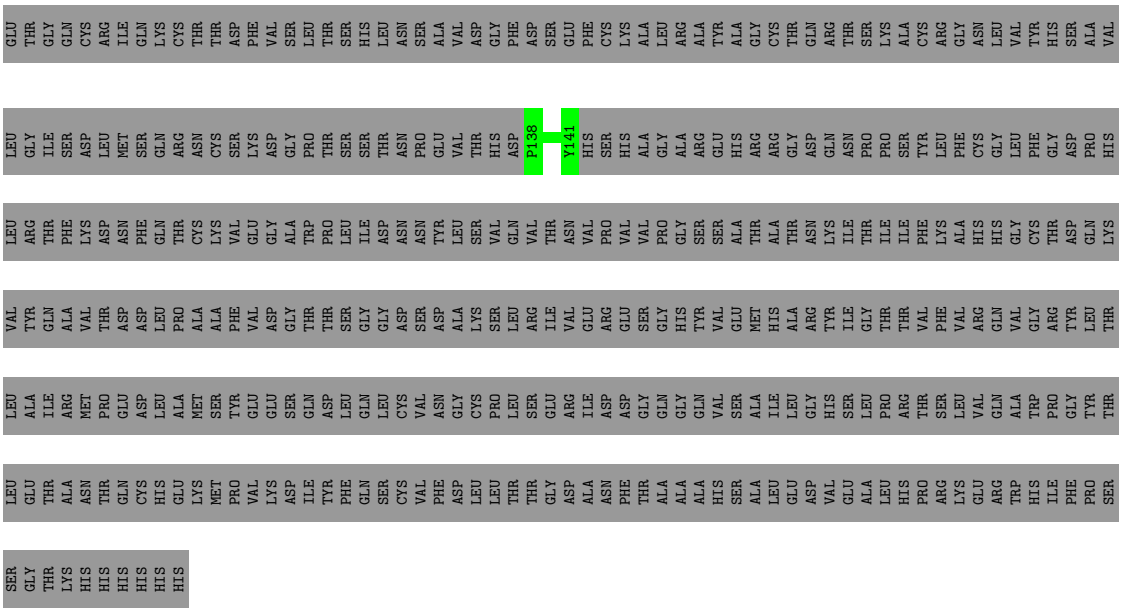
Chain W:





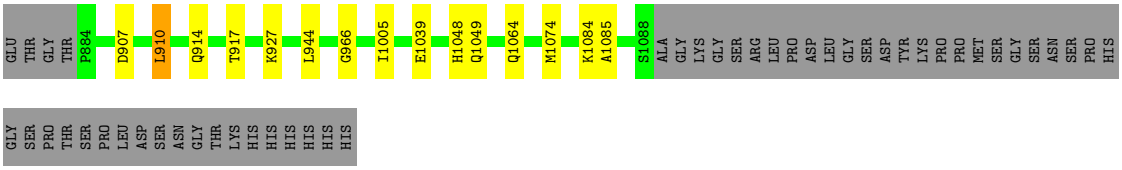
• Molecule 2: RGM domain family member B

Chain X: 99%



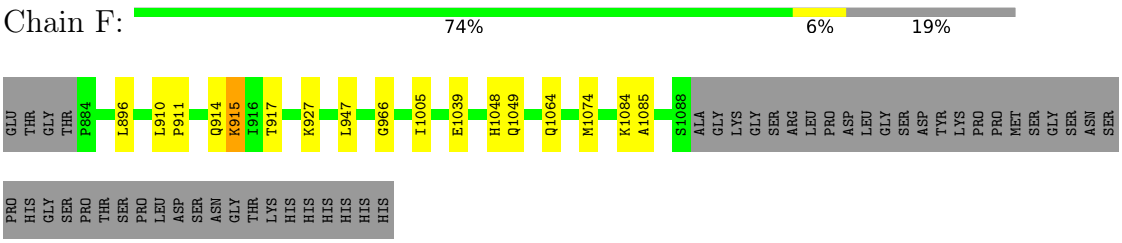
• Molecule 3: Neogenin

Chain E: 75% 6% 19%



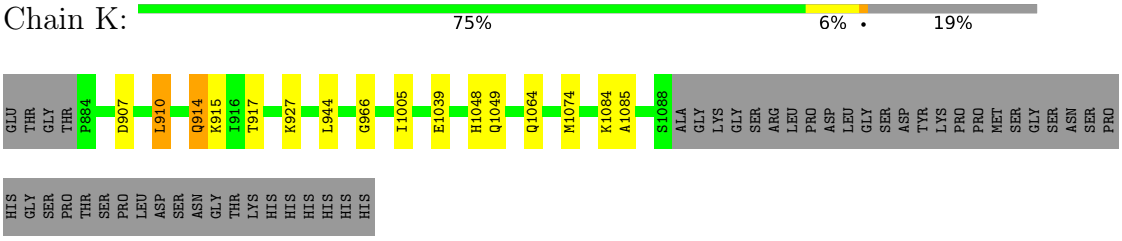
• Molecule 3: Neogenin

Chain F:



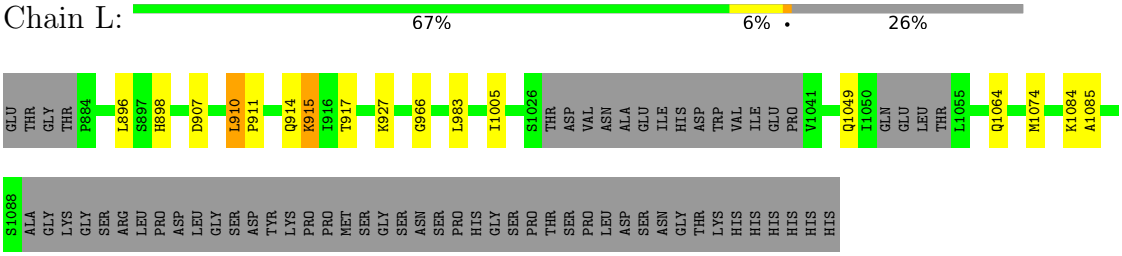
• Molecule 3: Neogenin

Chain K:



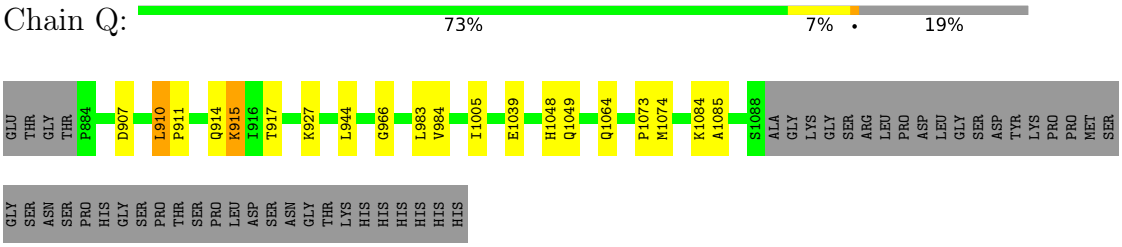
• Molecule 3: Neogenin

Chain L:



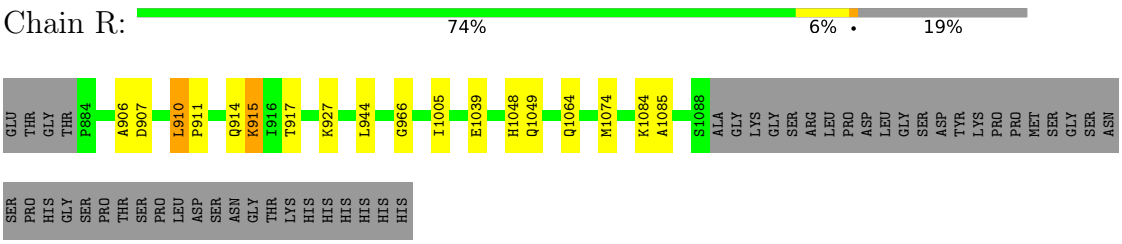
• Molecule 3: Neogenin

Chain Q:



• Molecule 3: Neogenin

Chain R:



4 Data and refinement statistics (i)

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 70.19 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (69.87-5.50) 99.8 (70.19-5.50)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 5.41Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, R_{free}	0.326 , 0.428 0.331 , 0.428	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)	0.36 , 500.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.106 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.80	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.*

[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	A	0.35	0/834	0.55	0/1131
1	B	0.37	0/849	0.57	0/1154
1	G	0.37	0/842	0.58	0/1143
1	H	0.35	0/832	0.55	0/1129
1	M	0.35	0/834	0.55	0/1132
1	N	0.37	0/852	0.58	0/1157
2	C	0.36	0/563	0.49	0/756
2	D	0.32	0/573	0.50	0/770
2	I	0.33	0/542	0.50	0/725
2	J	0.36	0/527	0.50	0/706
2	O	0.35	0/535	0.49	0/718
2	P	0.32	0/577	0.50	0/775
2	S	0.35	0/34	0.68	0/45
2	T	0.36	0/34	0.69	0/45
2	U	0.36	0/34	0.68	0/45
2	V	0.35	0/34	0.69	0/45
2	W	0.35	0/34	0.69	0/45
2	X	0.35	0/34	0.69	0/45
2	c	0.52	0/1243	0.73	0/1687
2	d	0.52	0/1244	0.73	0/1689
2	i	0.52	0/1216	0.74	0/1653
2	j	0.52	0/1236	0.73	0/1679
2	o	0.52	0/1232	0.74	0/1675
2	p	0.52	0/1237	0.73	0/1679
3	E	0.52	0/1646	0.68	0/2250
3	F	0.52	0/1639	0.68	0/2240
3	K	0.51	0/1647	0.68	0/2250
3	L	0.52	0/1466	0.69	0/1999
3	Q	0.52	0/1646	0.69	0/2248
3	R	0.52	0/1639	0.68	0/2242
All	All	0.47	0/25655	0.66	0/34857

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	A	813	0	754	4	0
1	B	828	0	785	7	0
1	G	821	0	770	7	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	3	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	0	0
2	d	1219	0	1182	0	0
2	i	1193	0	1142	0	0
2	j	1211	0	1164	0	0
2	o	1207	0	1160	0	0
2	p	1212	0	1167	0	0
3	E	1602	0	1584	9	0
3	F	1596	0	1578	13	0
3	K	1604	0	1599	12	0
3	L	1429	0	1416	11	0
3	Q	1603	0	1598	13	0
3	R	1596	0	1577	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	114	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.

All (114) 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:E:914:GLN:HB3	3:E:944:LEU:HD13	1.58	0.86
3:R:910:LEU:HD23	3:R:914:GLN:C	1.97	0.85
3:Q:910:LEU:HD23	3:Q:914:GLN:C	1.98	0.84
3:L:910:LEU:HD23	3:L:914:GLN:C	1.99	0.82
3:K:910:LEU:CD2	3:K:915:LYS:O	2.31	0.79
3:F:910:LEU:HD12	3:F:911:PRO:HD3	1.68	0.73
3:R:910:LEU:HD23	3:R:914:GLN:CA	2.21	0.70
3:Q:910:LEU:HD23	3:Q:914:GLN:CA	2.21	0.70
3:L:910:LEU:HD23	3:L:914:GLN:CA	2.22	0.69
3:K:910:LEU:HD23	3:K:914:GLN:C	2.13	0.68
3:K:910:LEU:HD21	3:K:915:LYS:O	1.94	0.66
3:K:914:GLN:OE1	3:K:914:GLN:N	2.30	0.64
3:Q:910:LEU:HD23	3:Q:914:GLN:HA	1.80	0.63
1:N:436:PRO:O	1:N:438:ARG:NH1	2.34	0.61
3:R:910:LEU:HD23	3:R:914:GLN:HA	1.81	0.61
1:G:436:PRO:O	1:G:438:ARG:NH1	2.34	0.61
3:F:910:LEU:HG	3:F:911:PRO:HD2	1.81	0.60
3:L:910:LEU:HD23	3:L:914:GLN:HA	1.81	0.60
1:B:436:PRO:O	1:B:438:ARG:NH1	2.34	0.60
3:Q:914:GLN:HB3	3:Q:944:LEU:HD13	1.82	0.60
3:R:914:GLN:HB3	3:R:944:LEU:HD13	1.84	0.59
3:Q:1039:GLU:HG2	3:Q:1048:HIS:NE2	2.18	0.59
3:R:1039:GLU:HG2	3:R:1048:HIS:NE2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:1039:GLU:HG2	3:K:1048:HIS:NE2	2.18	0.59
3:F:1039:GLU:HG2	3:F:1048:HIS:NE2	2.18	0.58
3:Q:1084:LYS:HG2	3:Q:1085:ALA:H	1.69	0.58
3:K:1084:LYS:HG2	3:K:1085:ALA:H	1.69	0.58
3:R:1084:LYS:HG2	3:R:1085:ALA:H	1.69	0.58
3:E:1084:LYS:HG2	3:E:1085:ALA:H	1.69	0.58
3:F:910:LEU:HD23	3:F:914:GLN:HA	1.86	0.58
3:E:1039:GLU:HG2	3:E:1048:HIS:NE2	2.18	0.57
3:L:1084:LYS:HG2	3:L:1085:ALA:H	1.68	0.57
3:F:1084:LYS:HG2	3:F:1085:ALA:H	1.69	0.57
3:K:1064:GLN:HB3	3:K:1074:MET:HG3	1.88	0.56
3:L:1064:GLN:HB3	3:L:1074:MET:HG3	1.88	0.56
3:R:1064:GLN:HB3	3:R:1074:MET:HG3	1.88	0.56
3:E:1064:GLN:HB3	3:E:1074:MET:HG3	1.88	0.55
3:Q:1064:GLN:HB3	3:Q:1074:MET:HG3	1.88	0.55
3:F:910:LEU:HD23	3:F:914:GLN:OE1	2.07	0.55
3:F:1064:GLN:HB3	3:F:1074:MET:HG3	1.88	0.54
3:K:910:LEU:HG	3:K:915:LYS:O	2.08	0.53
3:E:910:LEU:HD23	3:E:914:GLN:HA	1.90	0.53
1:N:438:ARG:HG3	1:N:440:HIS:CE1	2.44	0.52
1:B:438:ARG:HG3	1:B:440:HIS:CE1	2.44	0.51
1:G:438:ARG:HG3	1:G:440:HIS:CE1	2.44	0.51
3:K:910:LEU:CG	3:K:915:LYS:O	2.59	0.51
2:D:119:ARG:HA	4:D:1001:NAG:H82	1.94	0.50
2:P:119:ARG:HA	4:P:1001:NAG:H82	1.94	0.50
3:F:910:LEU:HG	3:F:911:PRO:CD	2.42	0.50
2:I:119:ARG:HA	4:I:1001:NAG:H82	1.94	0.49
1:H:442:GLU:OE1	1:H:470:ARG:NH1	2.45	0.49
3:E:910:LEU:HD23	3:E:914:GLN:C	2.33	0.49
2:J:88:TYR:O	2:J:92:THR:HG23	2.13	0.49
2:O:88:TYR:O	2:O:92:THR:HG23	2.13	0.48
1:G:438:ARG:HH21	1:G:441:LEU:HD11	1.79	0.48
2:C:88:TYR:O	2:C:92:THR:HG23	2.13	0.48
1:N:438:ARG:HH21	1:N:441:LEU:HD11	1.79	0.48
1:B:438:ARG:HH21	1:B:441:LEU:HD11	1.79	0.47
1:A:442:GLU:OE1	1:A:470:ARG:NH1	2.45	0.47
3:F:910:LEU:HD23	3:F:914:GLN:CA	2.45	0.47
3:L:898:HIS:CE1	3:Q:984:VAL:CG1	2.98	0.46
1:G:438:ARG:HG2	1:G:441:LEU:HG	1.98	0.46
3:L:1005:ILE:HG12	3:L:1049:GLN:HG2	1.98	0.46
1:B:438:ARG:HG2	1:B:441:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:71:ASN:HB3	2:C:74:VAL:HG23	1.97	0.46
3:K:1005:ILE:HG12	3:K:1049:GLN:HG2	1.98	0.46
3:Q:1005:ILE:HG12	3:Q:1049:GLN:HG2	1.98	0.46
3:E:1005:ILE:HG12	3:E:1049:GLN:HG2	1.97	0.46
3:Q:911:PRO:HB2	3:Q:915:LYS:HZ3	1.79	0.45
3:R:1005:ILE:HG12	3:R:1049:GLN:HG2	1.98	0.45
1:M:442:GLU:OE1	1:M:470:ARG:NH1	2.45	0.45
1:N:438:ARG:HG2	1:N:441:LEU:HG	1.98	0.45
3:F:1005:ILE:HG12	3:F:1049:GLN:HG2	1.98	0.44
1:H:438:ARG:H	1:H:438:ARG:HG2	1.44	0.44
1:B:441:LEU:HD13	1:B:500:CYS:SG	2.58	0.44
2:J:71:ASN:HB3	2:J:74:VAL:HG23	1.98	0.44
1:M:417:TRP:CZ3	2:O:101:GLY:HA2	2.52	0.44
1:N:441:LEU:HD13	1:N:500:CYS:SG	2.57	0.44
1:A:417:TRP:CZ3	2:C:101:GLY:HA2	2.52	0.44
3:E:910:LEU:HD23	3:E:914:GLN:CA	2.47	0.44
1:H:417:TRP:CZ3	2:J:101:GLY:HA2	2.52	0.44
1:G:441:LEU:HD13	1:G:500:CYS:SG	2.58	0.43
3:F:911:PRO:HB2	3:F:915:LYS:HE3	2.00	0.43
3:L:911:PRO:HB2	3:L:915:LYS:HZ3	1.84	0.43
3:L:983:LEU:HD11	3:Q:983:LEU:CD1	2.49	0.43
2:I:88:TYR:O	2:I:92:THR:HG23	2.19	0.43
3:F:914:GLN:HA	3:F:914:GLN:OE1	2.19	0.42
2:P:88:TYR:O	2:P:92:THR:HG23	2.19	0.42
2:D:88:TYR:O	2:D:92:THR:HG23	2.19	0.42
1:M:438:ARG:HD3	2:P:64:VAL:HG11	2.02	0.42
3:R:907:ASP:HB3	3:R:910:LEU:HB2	2.02	0.42
1:A:438:ARG:HD3	2:D:64:VAL:HG11	2.02	0.42
3:E:907:ASP:HB3	3:E:910:LEU:HB2	2.02	0.41
1:G:422:LEU:HD23	1:G:422:LEU:HA	1.87	0.41
1:H:438:ARG:HD3	2:I:64:VAL:HG11	2.02	0.41
3:L:907:ASP:HB3	3:L:910:LEU:HB2	2.02	0.41
1:N:438:ARG:HG2	1:N:438:ARG:H	1.66	0.41
1:B:396:LEU:HD22	2:C:71:ASN:HD21	1.85	0.41
2:D:115:LEU:HD23	2:D:115:LEU:HA	1.84	0.41
3:K:907:ASP:HB3	3:K:910:LEU:HB2	2.02	0.41
1:N:396:LEU:HD23	1:N:396:LEU:HA	1.90	0.41
1:N:396:LEU:HD22	2:O:71:ASN:HD21	1.86	0.41
1:G:396:LEU:HD22	2:J:71:ASN:HD21	1.86	0.41
3:Q:907:ASP:HB3	3:Q:910:LEU:HB2	2.02	0.41
3:R:914:GLN:CB	3:R:944:LEU:HD13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:896:LEU:HB3	3:Q:1073:PRO:HB3	2.03	0.40
1:A:438:ARG:H	1:A:438:ARG:HG2	1.43	0.40
2:C:103:LEU:HD23	2:C:103:LEU:HA	1.89	0.40
1:B:417:TRP:CZ3	2:D:101:GLY:HA2	2.57	0.40
3:R:911:PRO:HB2	3:R:915:LYS:HZ3	1.86	0.40
2:D:116:MET:HE3	2:D:121:CYS:HB2	2.02	0.40
3:F:896:LEU:HD12	3:F:947:LEU:HD11	2.04	0.40
3:R:906:ALA:HB1	3:R:914:GLN:NE2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	29	69
3	F	203/253 (80%)	192 (95%)	10 (5%)	1 (0%)	29	69
3	K	203/253 (80%)	192 (95%)	10 (5%)	1 (0%)	29	69
3	L	181/253 (72%)	170 (94%)	10 (6%)	1 (1%)	25	65
3	Q	203/253 (80%)	192 (95%)	10 (5%)	1 (0%)	29	69
3	R	203/253 (80%)	192 (95%)	10 (5%)	1 (0%)	29	69
All	All	3165/8898 (36%)	3011 (95%)	148 (5%)	6 (0%)	47	81

All (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
3	R	966	GLY

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	91/107 (85%)	89 (98%)	2 (2%)	52	71
1	B	94/107 (88%)	93 (99%)	1 (1%)	73	84
1	G	92/107 (86%)	91 (99%)	1 (1%)	73	84
1	H	90/107 (84%)	88 (98%)	2 (2%)	52	71
1	M	91/107 (85%)	89 (98%)	2 (2%)	52	71
1	N	94/107 (88%)	93 (99%)	1 (1%)	73	84
2	C	62/317 (20%)	62 (100%)	0	100	100
2	D	64/317 (20%)	64 (100%)	0	100	100
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%)	64 (100%)	0	100	100
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
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%)	129 (96%)	6 (4%)	28	53
2	d	135/317 (43%)	129 (96%)	6 (4%)	28	53
2	i	131/317 (41%)	126 (96%)	5 (4%)	33	57
2	j	133/317 (42%)	128 (96%)	5 (4%)	33	57
2	o	133/317 (42%)	128 (96%)	5 (4%)	33	57
2	p	133/317 (42%)	127 (96%)	6 (4%)	27	53
3	E	178/222 (80%)	175 (98%)	3 (2%)	60	78
3	F	177/222 (80%)	174 (98%)	3 (2%)	60	78
3	K	179/222 (81%)	175 (98%)	4 (2%)	52	71
3	L	156/222 (70%)	152 (97%)	4 (3%)	46	67
3	Q	179/222 (81%)	175 (98%)	4 (2%)	52	71
3	R	177/222 (80%)	173 (98%)	4 (2%)	50	70
All	All	2786/7680 (36%)	2722 (98%)	64 (2%)	50	70

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	399	ARG
1	A	438	ARG
1	B	438	ARG
3	E	910	LEU
3	E	917	THR
3	E	927	LYS
3	F	915	LYS
3	F	917	THR
3	F	927	LYS
1	G	438	ARG
1	H	399	ARG
1	H	438	ARG
3	K	910	LEU
3	K	914	GLN
3	K	917	THR
3	K	927	LYS
3	L	910	LEU
3	L	915	LYS
3	L	917	THR
3	L	927	LYS
1	M	399	ARG
1	M	438	ARG
1	N	438	ARG
3	Q	910	LEU
3	Q	915	LYS
3	Q	917	THR
3	Q	927	LYS
3	R	910	LEU
3	R	915	LYS
3	R	917	THR
3	R	927	LYS
2	c	172	ARG
2	c	177	ASN
2	c	252	ASP
2	c	257	SER
2	c	261	VAL
2	c	269	VAL
2	d	172	ARG
2	d	177	ASN
2	d	252	ASP
2	d	257	SER
2	d	261	VAL

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Mol	Chain	Res	Type
2	d	269	VAL
2	i	177	ASN
2	i	252	ASP
2	i	257	SER
2	i	261	VAL
2	i	269	VAL
2	j	177	ASN
2	j	252	ASP
2	j	257	SER
2	j	261	VAL
2	j	269	VAL
2	o	177	ASN
2	o	252	ASP
2	o	257	SER
2	o	261	VAL
2	o	269	VAL
2	p	172	ARG
2	p	177	ASN
2	p	252	ASP
2	p	257	SER
2	p	261	VAL
2	p	269	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	F	2001	3	14,14,15	0.32	0	17,19,21	0.71	1 (5%)
4	NAG	D	1001	2	14,14,15	0.46	0	17,19,21	0.66	0
4	NAG	P	1001	2	14,14,15	0.49	0	17,19,21	0.69	0
4	NAG	L	2001	3	14,14,15	0.28	0	17,19,21	0.73	1 (5%)
4	NAG	I	1001	2	14,14,15	0.48	0	17,19,21	0.68	0
4	NAG	R	2001	3	14,14,15	0.28	0	17,19,21	0.70	1 (5%)
4	NAG	Q	2001	3	14,14,15	0.28	0	17,19,21	0.74	1 (5%)
4	NAG	E	2001	3	14,14,15	0.31	0	17,19,21	0.71	1 (5%)
4	NAG	K	2001	3	14,14,15	0.31	0	17,19,21	0.73	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	F	2001	3	-	0/6/23/26	0/1/1/1
4	NAG	D	1001	2	-	0/6/23/26	0/1/1/1
4	NAG	P	1001	2	-	0/6/23/26	0/1/1/1
4	NAG	L	2001	3	-	0/6/23/26	0/1/1/1
4	NAG	I	1001	2	-	0/6/23/26	0/1/1/1
4	NAG	R	2001	3	-	0/6/23/26	0/1/1/1
4	NAG	Q	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	K	2001	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Q	2001	NAG	C1-O5-C5	2.83	116.02	112.19
4	L	2001	NAG	C1-O5-C5	2.75	115.92	112.19
4	K	2001	NAG	C1-O5-C5	2.71	115.87	112.19
4	F	2001	NAG	C1-O5-C5	2.66	115.80	112.19
4	E	2001	NAG	C1-O5-C5	2.65	115.78	112.19
4	R	2001	NAG	C1-O5-C5	2.61	115.73	112.19

There are no chirality outliers.

There are no torsion outliers.

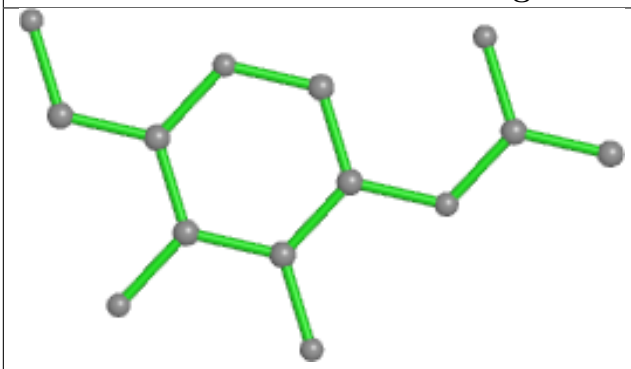
There are no ring outliers.

3 monomers are involved in 3 short contacts:

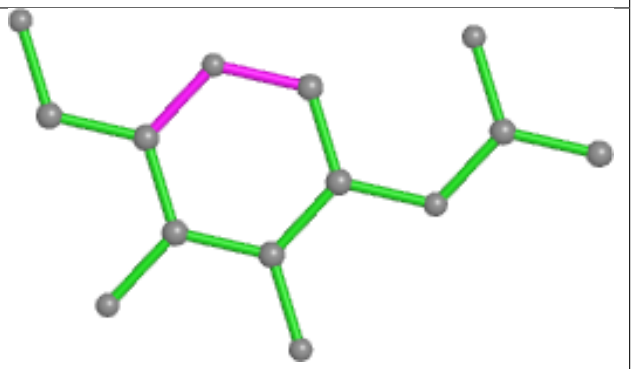
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1001	NAG	1	0
4	P	1001	NAG	1	0
4	I	1001	NAG	1	0

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 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.

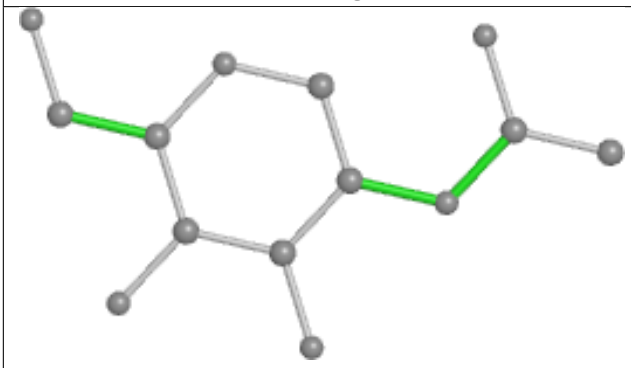
Ligand NAG F 2001



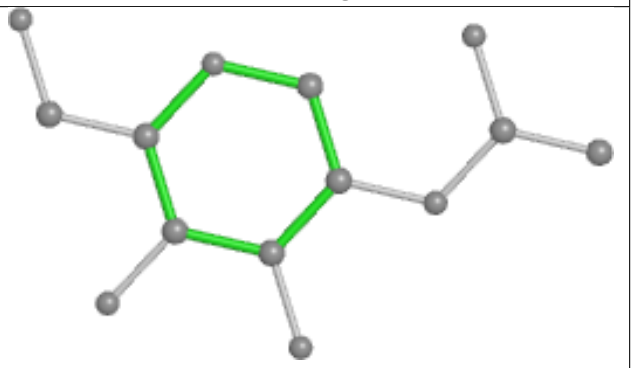
Bond lengths



Bond angles

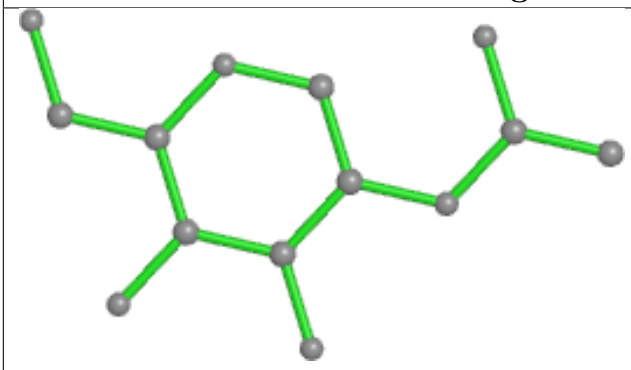


Torsions

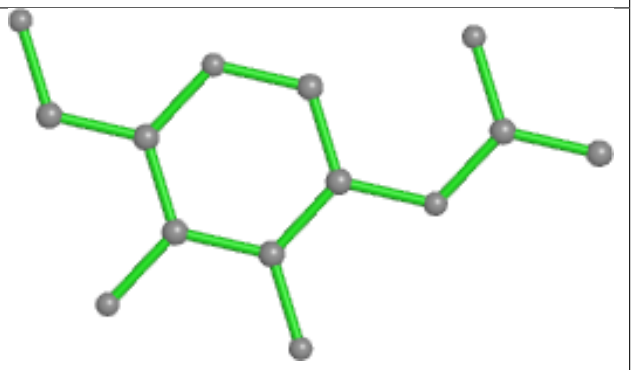


Rings

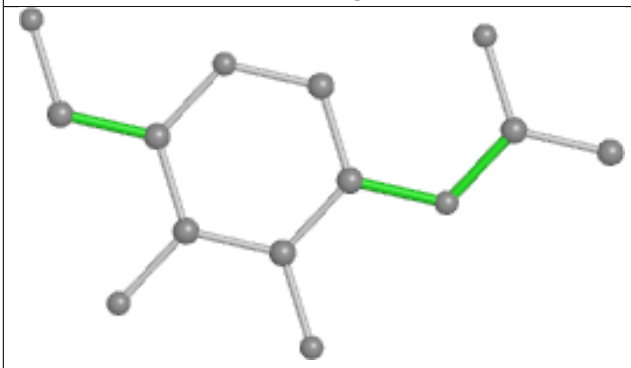
Ligand NAG D 1001



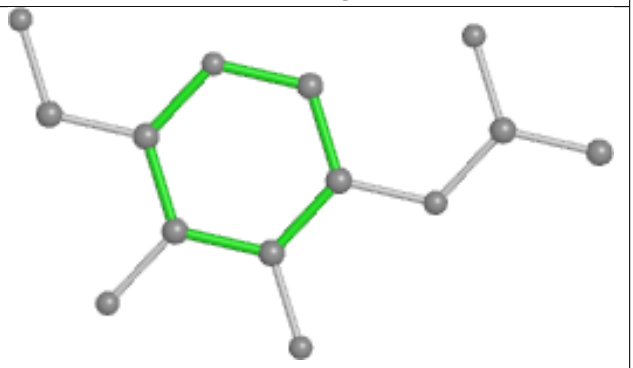
Bond lengths



Bond angles

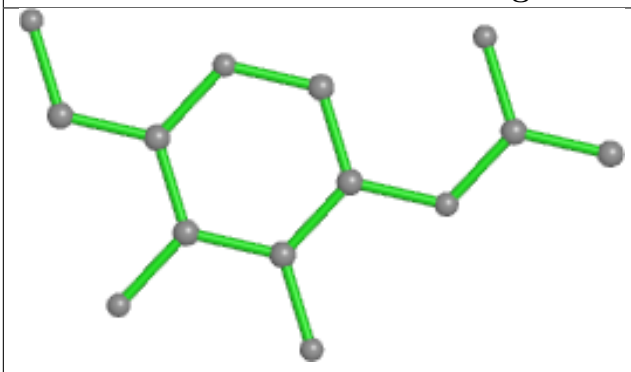


Torsions

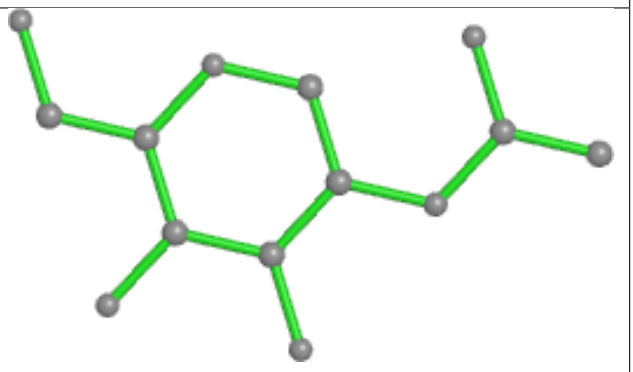


Rings

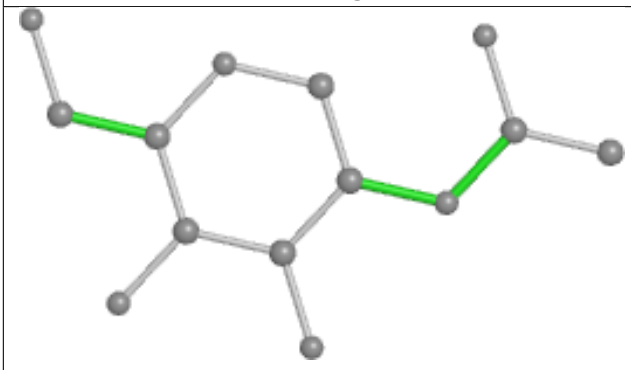
Ligand NAG P 1001



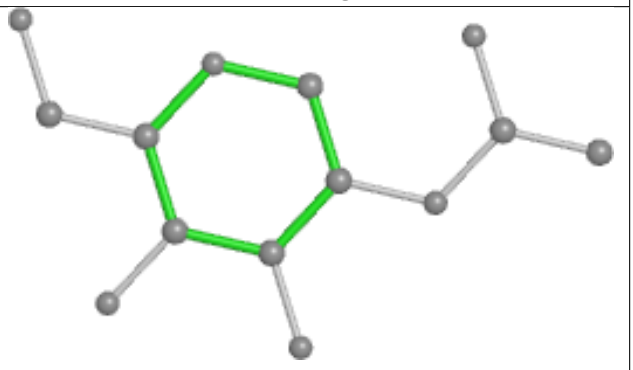
Bond lengths



Bond angles

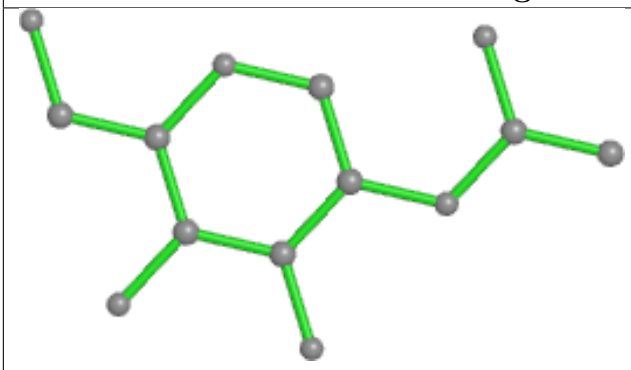


Torsions

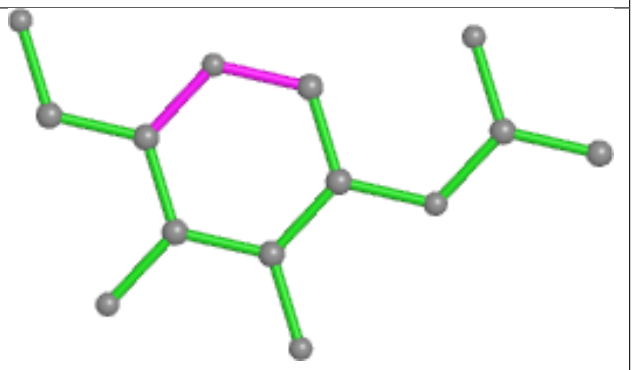


Rings

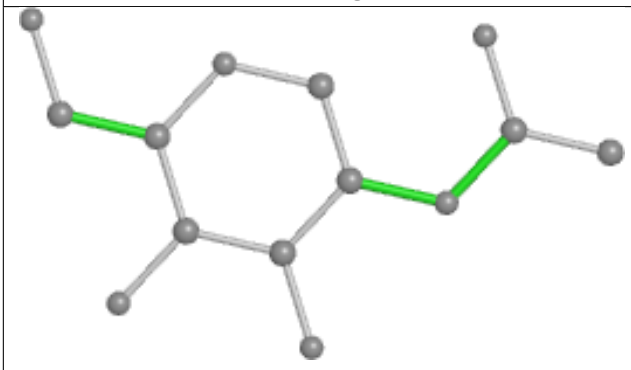
Ligand NAG L 2001



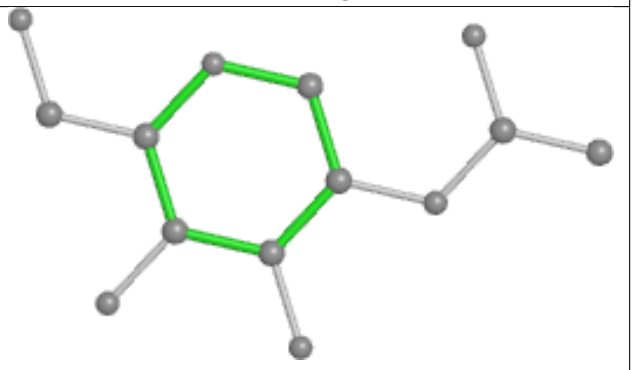
Bond lengths



Bond angles

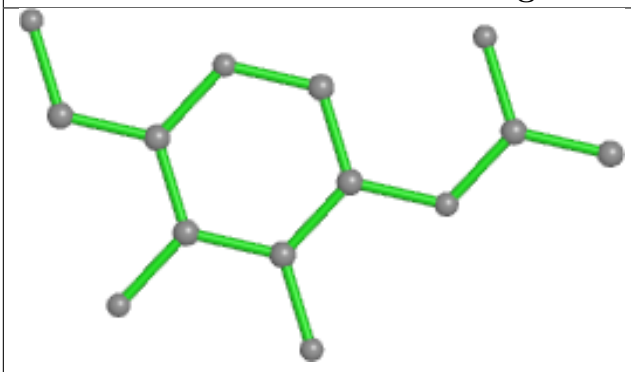


Torsions

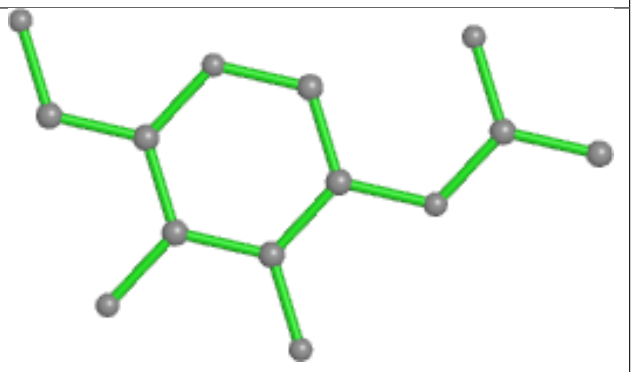


Rings

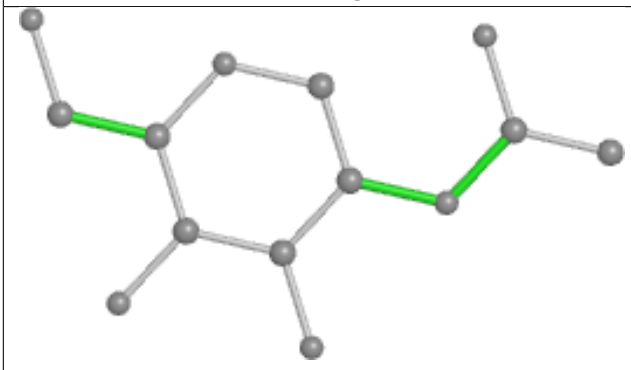
Ligand NAG I 1001



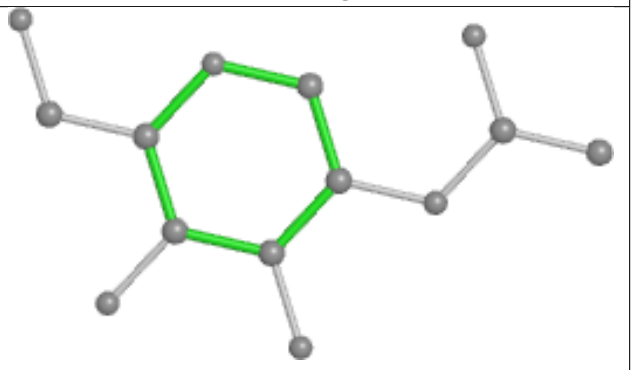
Bond lengths



Bond angles

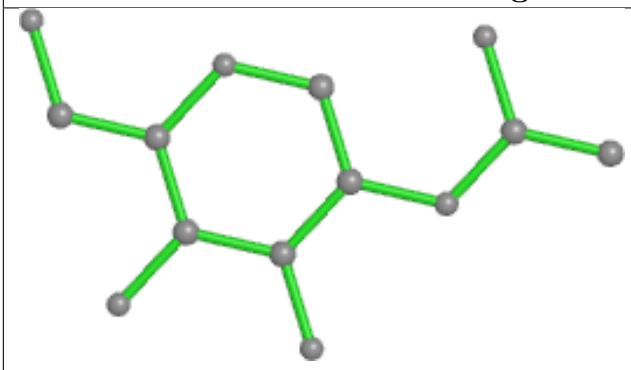


Torsions

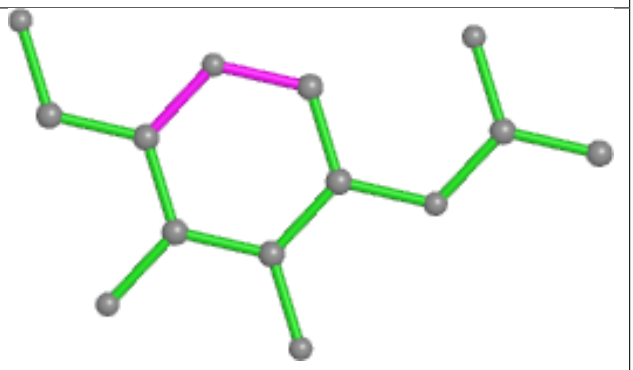


Rings

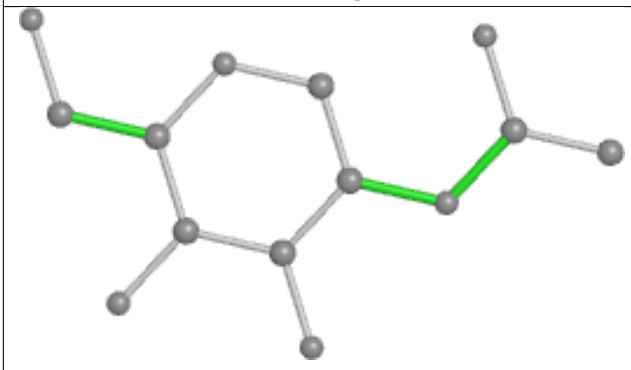
Ligand NAG R 2001



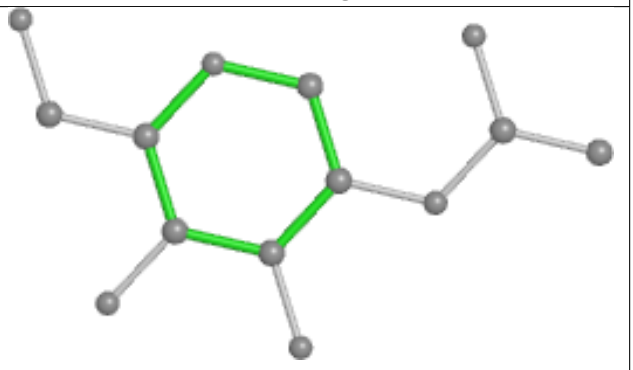
Bond lengths



Bond angles

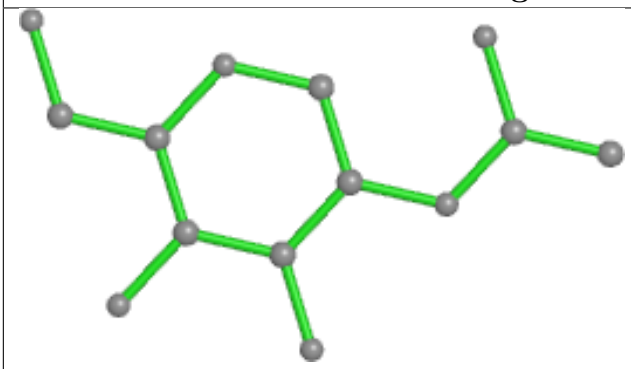


Torsions

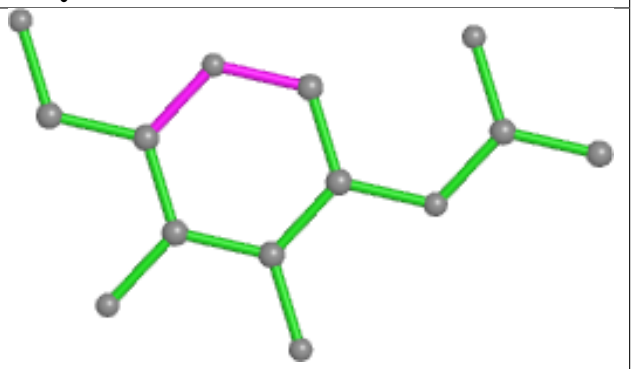


Rings

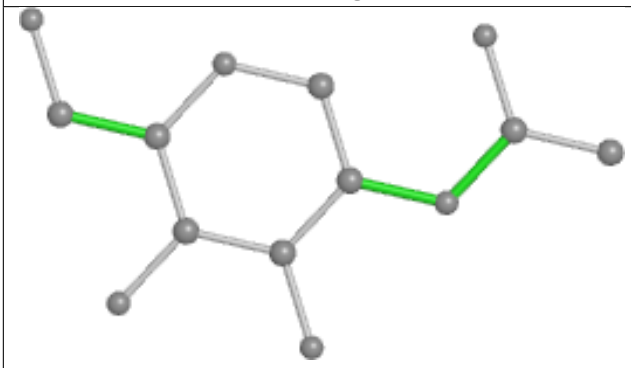
Ligand NAG Q 2001



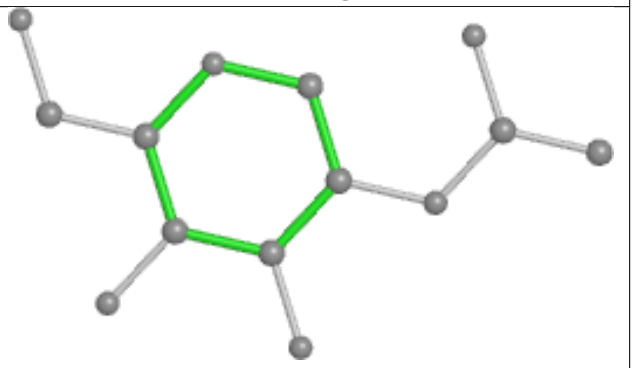
Bond lengths



Bond angles

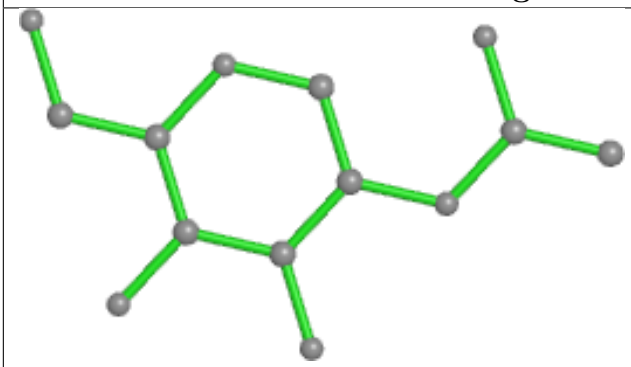


Torsions

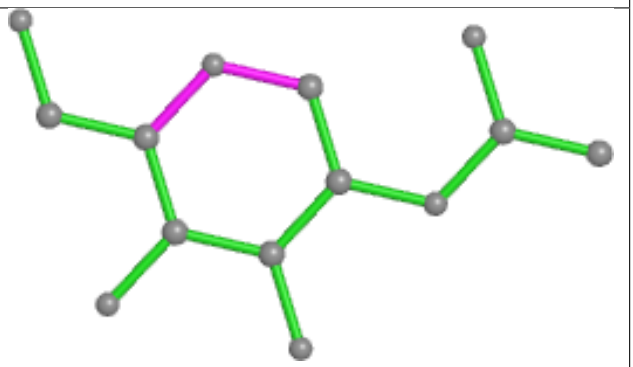


Rings

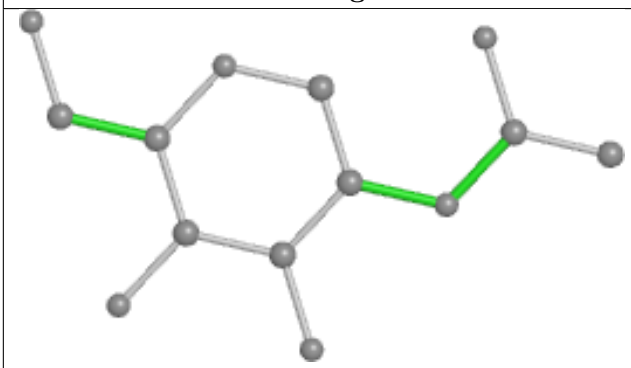
Ligand NAG E 2001



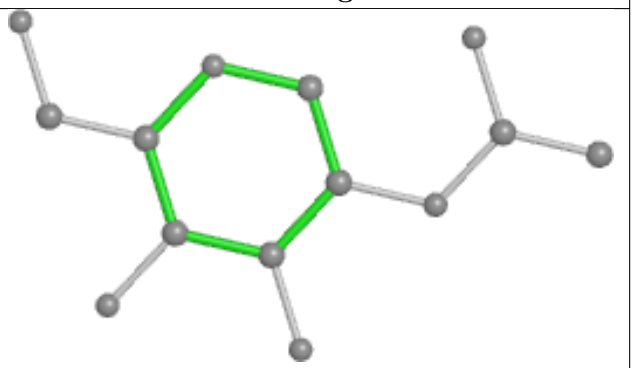
Bond lengths



Bond angles

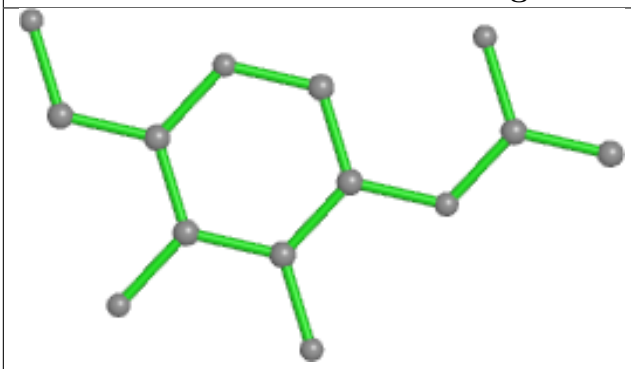


Torsions

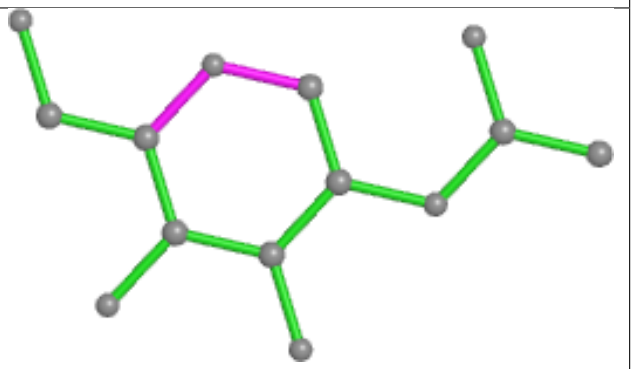


Rings

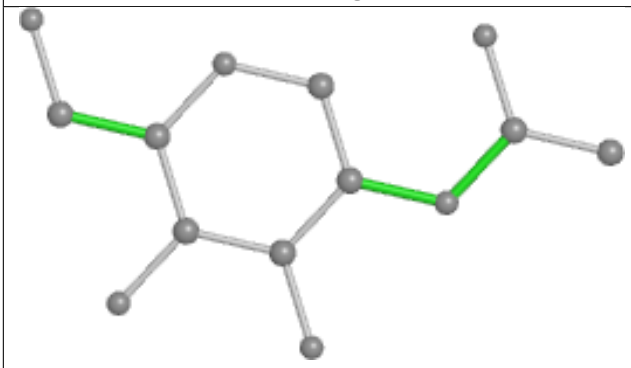
Ligand NAG K 2001



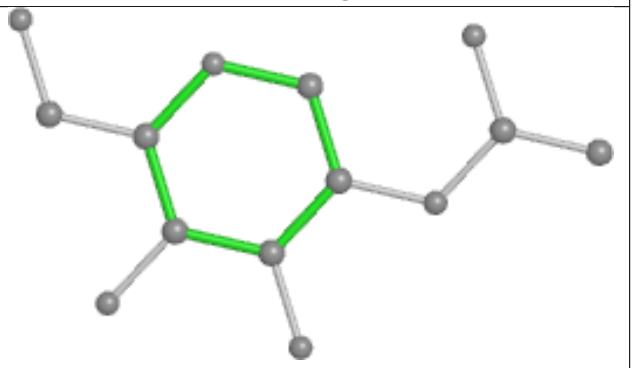
Bond lengths



Bond angles



Torsions



Rings

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

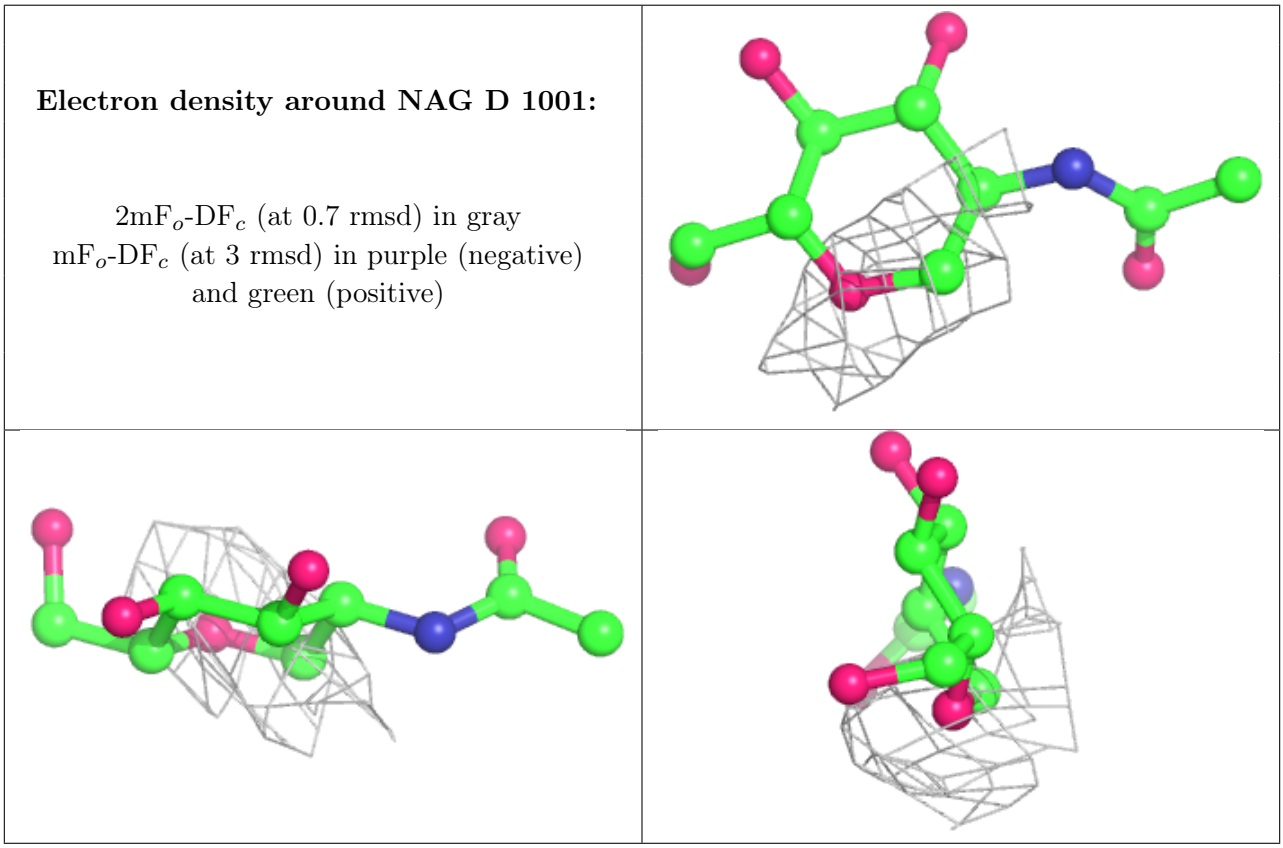
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

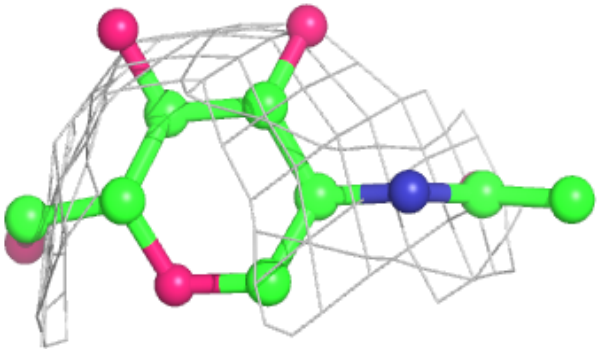
Electron density around NAG D 1001:

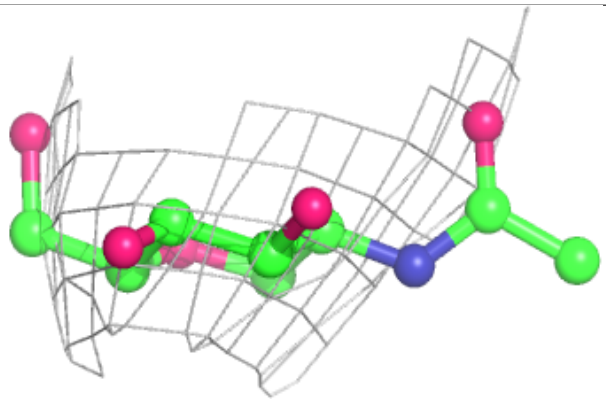
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

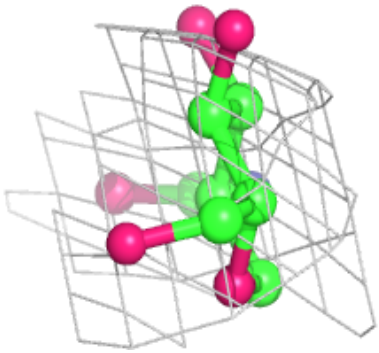


Electron density around NAG E 2001:

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

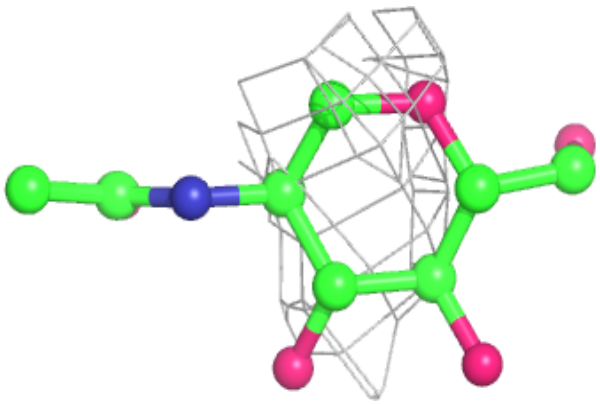


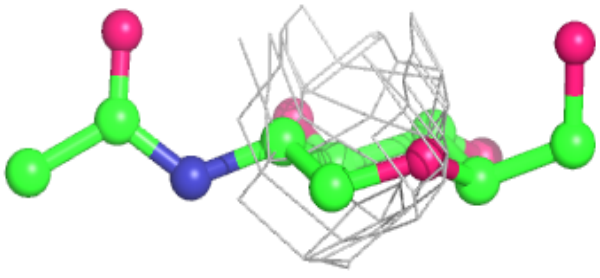


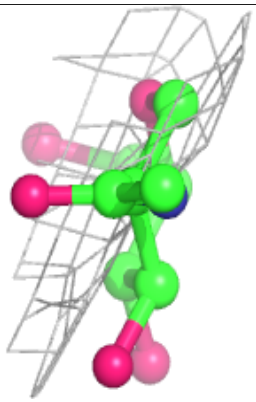


Electron density around NAG F 2001:

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

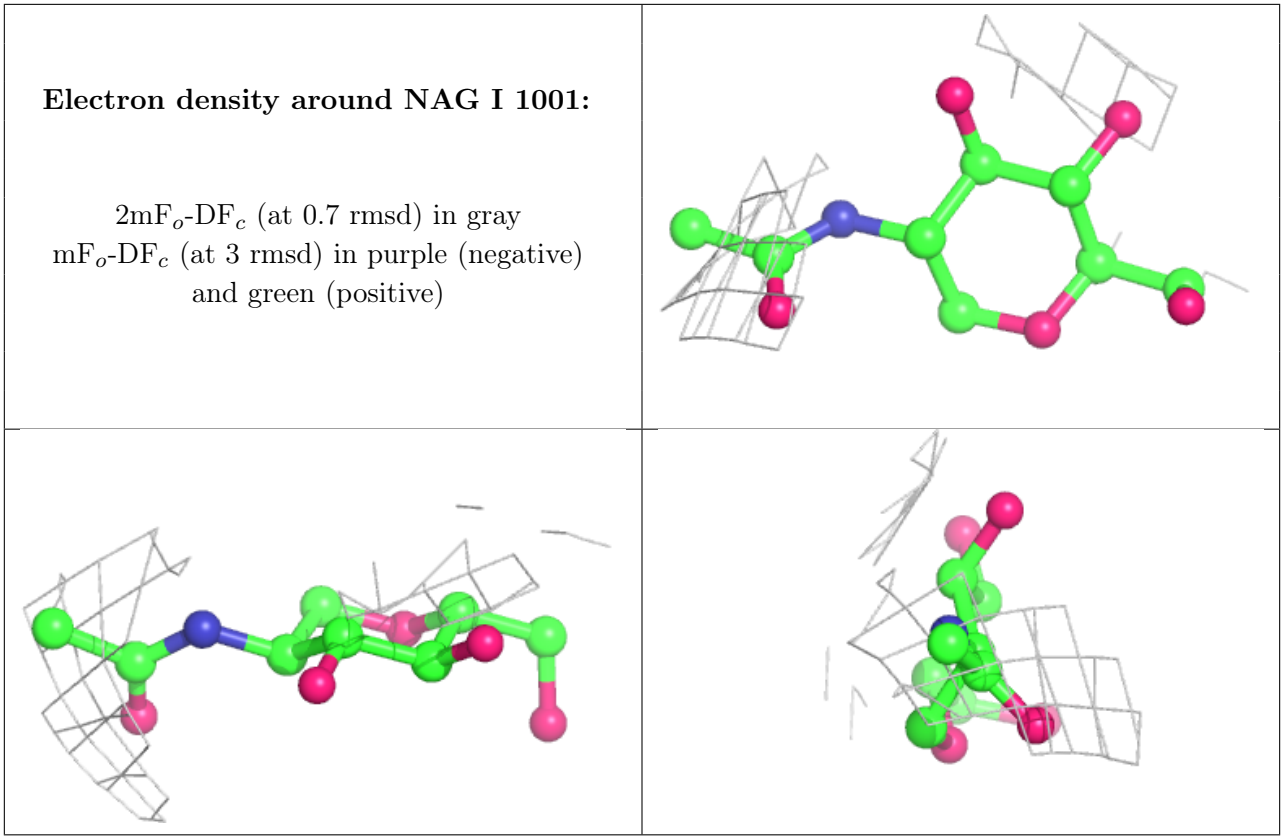






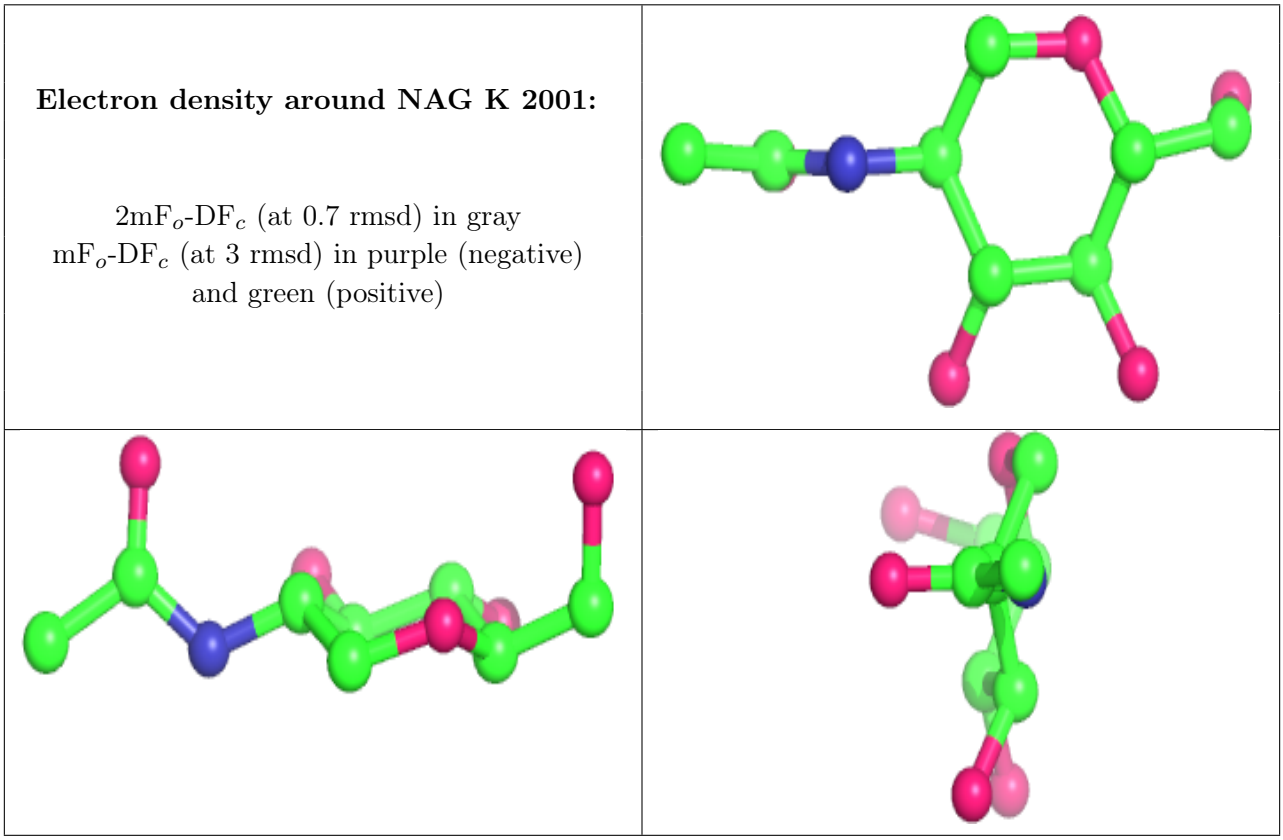
Electron density around NAG I 1001:

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



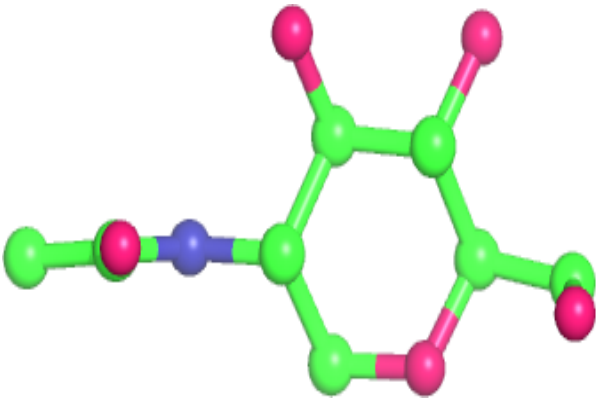
Electron density around NAG K 2001:

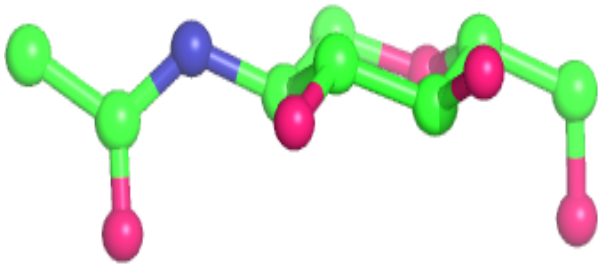
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

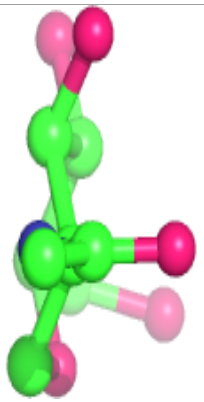


Electron density around NAG L 2001:

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

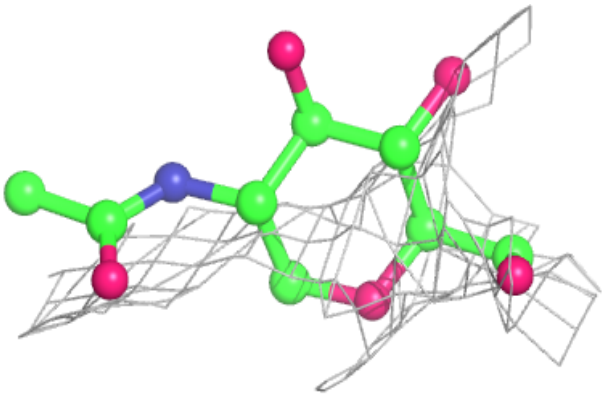


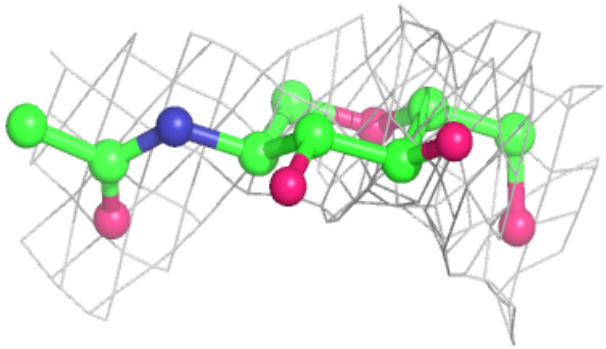


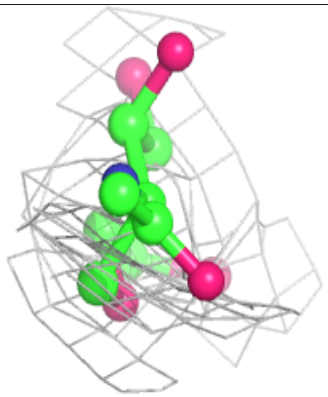


Electron density around NAG P 1001:

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

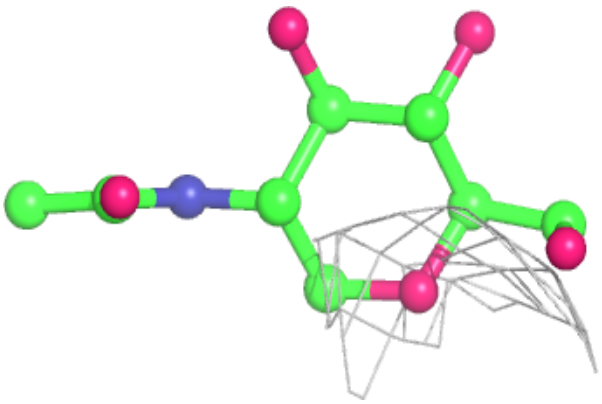


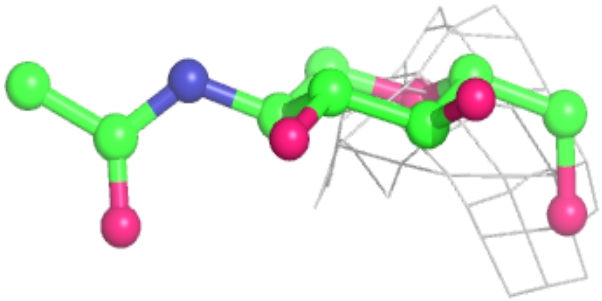


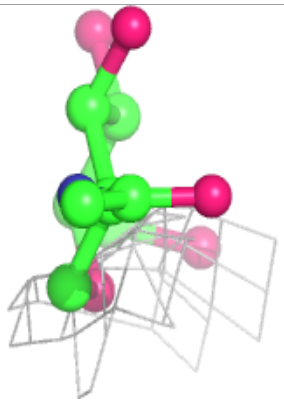


Electron density around NAG Q 2001:

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

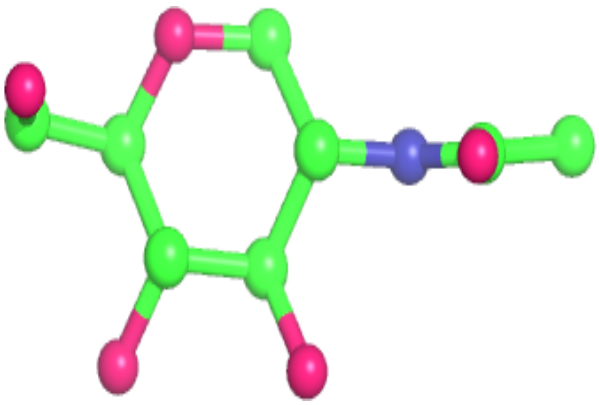


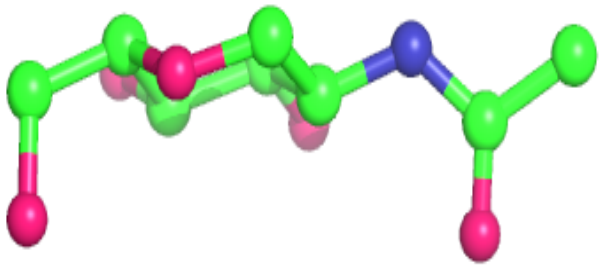


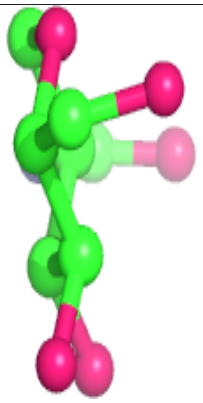


Electron density around NAG R 2001:

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







6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.