



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:48 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 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	:	4-5-2 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

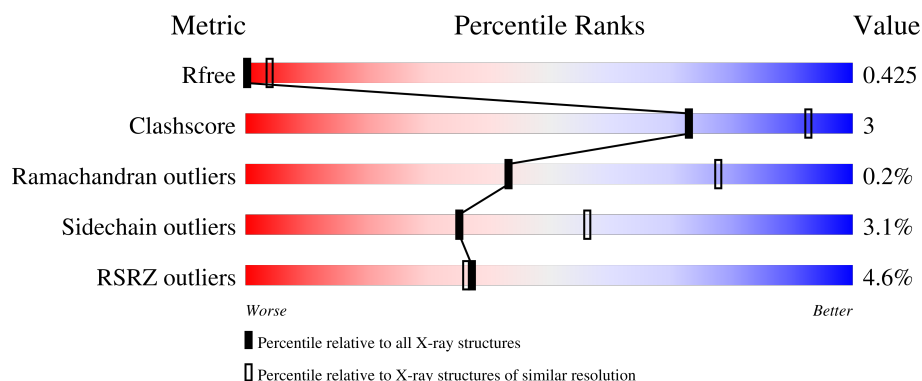
1 Overall quality at a glance

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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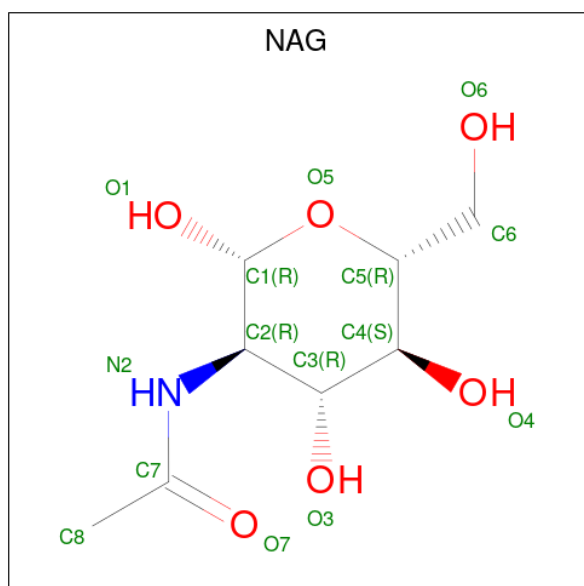
Chain	Residue	Modelled	Actual	Comment	Reference
F	1129	HIS	-	expression tag	UNP P97798
F	1130	HIS	-	expression tag	UNP P97798
F	1131	HIS	-	expression tag	UNP P97798
F	1132	HIS	-	expression tag	UNP P97798
K	880	GLU	-	expression tag	UNP P97798
K	881	THR	-	expression tag	UNP P97798
K	882	GLY	-	expression 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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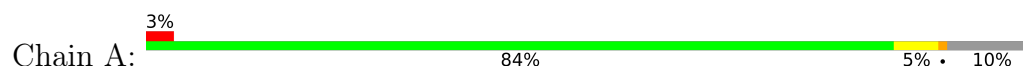
Continued from previous page...

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		

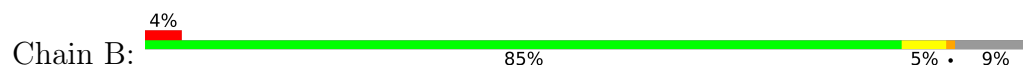
3 Residue-property plots [i](#)

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.

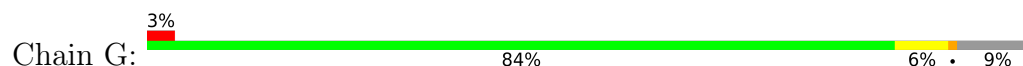
- Molecule 1: Growth/differentiation factor 5



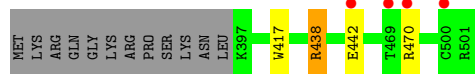
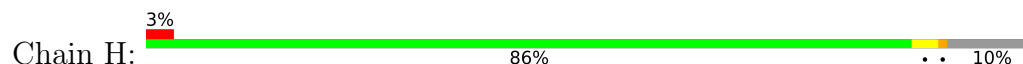
- Molecule 1: Growth/differentiation factor 5



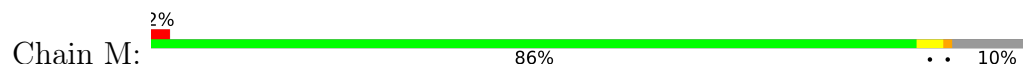
- Molecule 1: Growth/differentiation factor 5



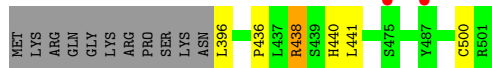
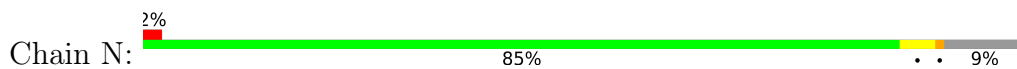
- Molecule 1: Growth/differentiation factor 5



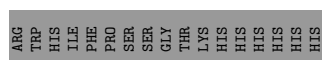
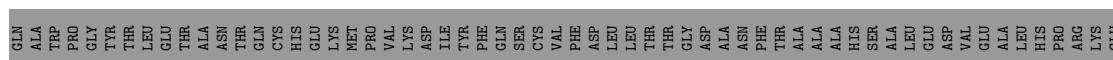
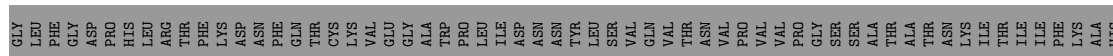
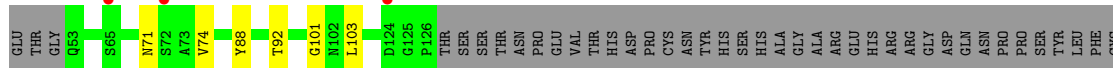
- Molecule 1: Growth/differentiation factor 5



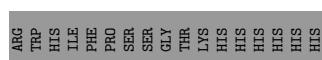
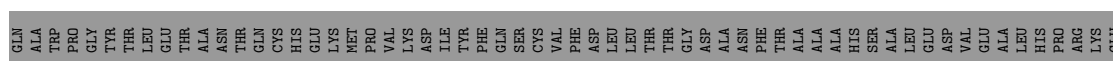
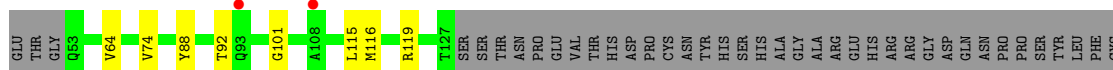
- Molecule 1: Growth/differentiation factor 5



- Molecule 2: RGM domain family member B



- Molecule 2: RGM domain family member B



- Molecule 2: RGM domain family member B



[illegible]

- Molecule 2: RGM domain family member B



GLU	THR	G52	V64	H69	A73	D75	E90	Y98	T92	Q93	S113	R119	P126	T127	SER	SER	THR	ASN	PRO	GLU	VAL	THR	THR	HIS	ASP	PRO	CYS	ASN	TYR	HIS	SER	HIS	ALA	GLY	ALA	ARG	GLU	HIS	ARG	ARG	ASP	ASN	PRO	PRO	SER	TYR	LEU	DEU
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CYS GLY LEU LEU PHE GLY ASP PRO HIS LEU LEU ARG THR PHE LYS ASP ASN PHE GLN THR CYS LYS VAL GLU GLY ALA ALA TRP PRO LEU LEU ILE ASP ASN ASN TYR SER SER VAL GLN VAL THR THR ASN VAL VAL VAL VAL VAL VAL GLY SER SER SER ALA THR ALA THR THR ASN LYS LYS LLE THR LLE LLE PHE LYS LYS

[illegible]

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

VAL	GLN	ALA	TRP	PRO	GLY	THR	LEU	GLU	THR	ALA	ASN	THR	GLN	CYS	GLY	GLU	HIS	MET	PRO	VAL	LYS	ASP	ILE	TYR	PHE	GLN	SER	CYS	VAL	PHE	ASP	LEU	LEU	THR	THR	GLY	ASP	ALA	ALA	ASN	PHE	THR	ALA	ALA	HIS	SER	ALA	LEU	GLU	ASP	VAL	VAL	GLU	ALA	ARG	LYS
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GLU
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- Molecule 2: RGM domain family member B



GLU	THR	GLY	GLN	CYS	ARG	ILE	GLN	LYS	THR	THR	ASP	PHE	VAL	SER	LEU	ASN	SER	ALA	VAL	ASP	GLY	PHE	ASP	SER	GLU	PHE	CYS	LYS	ALA	LEU	ARG	ALA	TYR	ALA	GLY	CYS	THR	LYS	SER	THR	THR	THR	ARG	CYS	ARG	GLY	ASN	LEU	VAL	TYR	HIS	SER	ALA	VAL
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TYR
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ALA
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ALA
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ARG
GLU
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ARG
GLY
ASP
GLN
ASN
PRO
ASP
P158
L161
P162
G167
ASP
P169
R172
P175

N177	F178	S196	V205	T213	I219	D228	L239	T248	D252	S257	I260	V261	E262	ARG	GLU	GLY	SER	GLY	HIS	Y268	V269	E270	L289	R294	E297	R321	ILE	ASP	ASP	GLY	GLN	GLY	GLN	VAL	SER	ALA	ILE	LEU	GLY	HIS	SER	LEU	PRO	ARG	THR	FER
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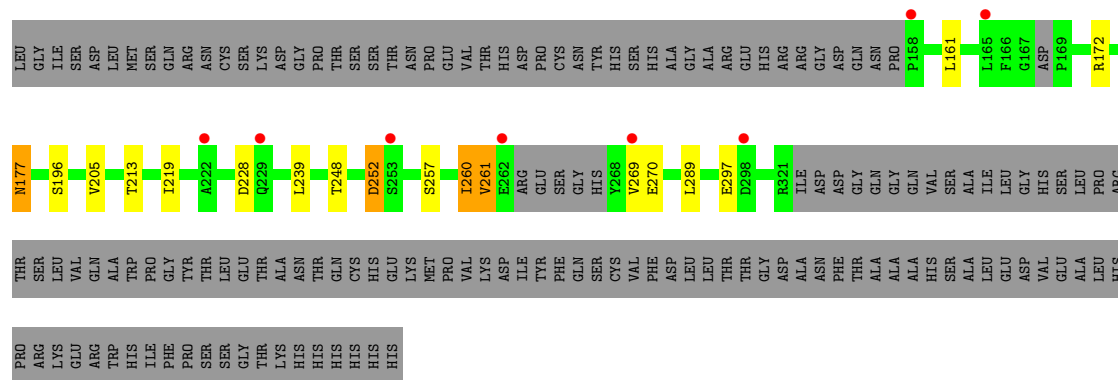
LEU
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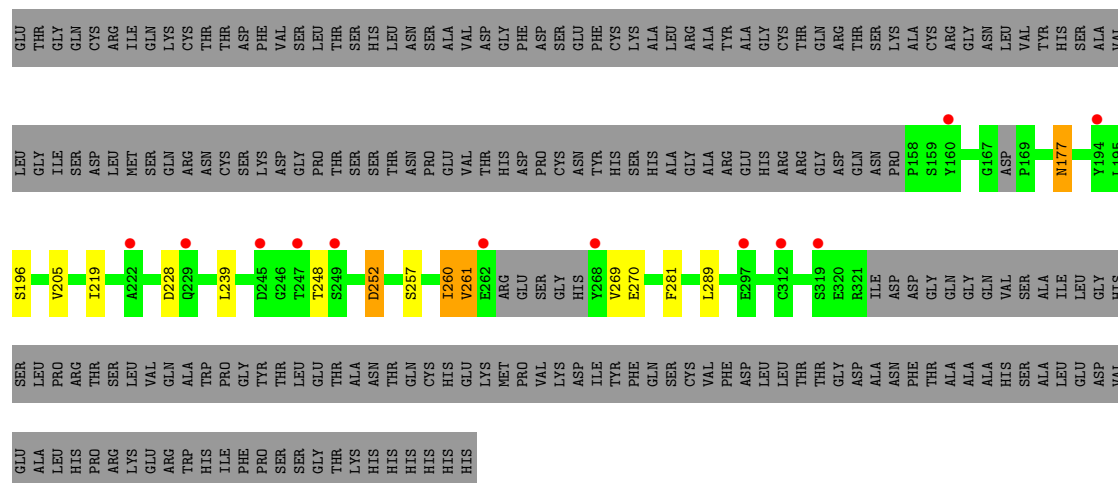
- Molecule 2: RGM domain family member B



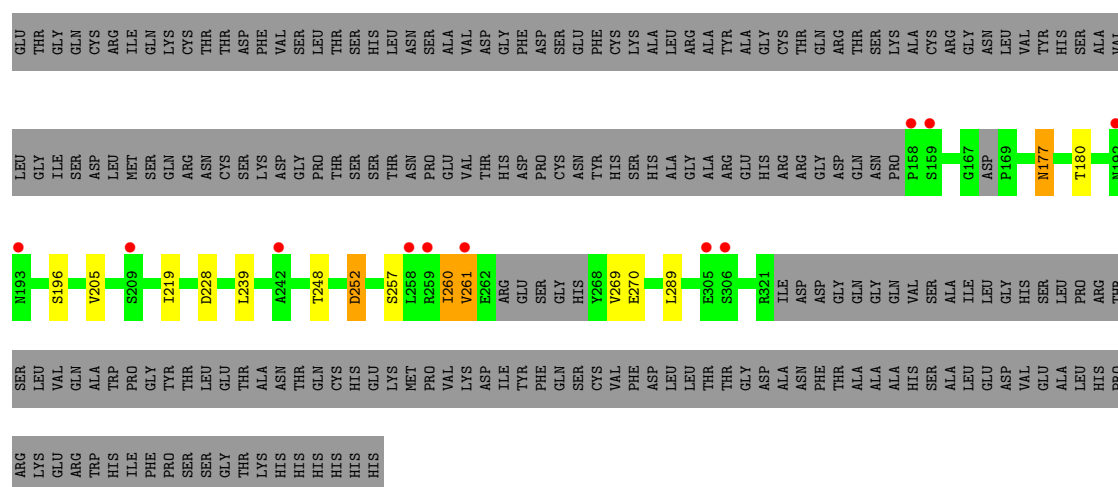
GLU	THR	GLY	GLN	CYS	ARG	ILE	GLN	CYS	THR	THR	ASP	ASP	PHE	VAL	SER	LEU	THR	SER	HIS	LEU	ASN	SER	ALA	VAL	ASP	GLY	PHE	ASP	PHE	SER	GLU	CYS	LYS	ALA	LEU	ARG	ALA	ALA	ALA	GLY	CYS	THR	THR	GLN	ARG	THR	THR	SER	LYS	SER	ALA	CYS	ARG	GLY	ASN	LEU	VAL	THR	VAL	HIS	SER	SER	ALA	VAL
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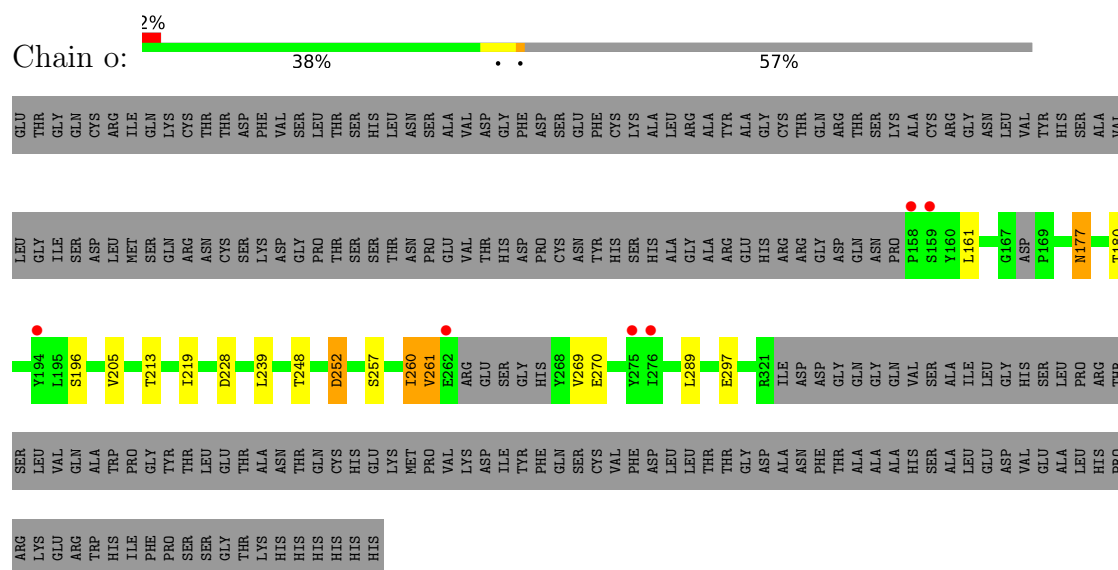
• Molecule 2: RGM domain family member B



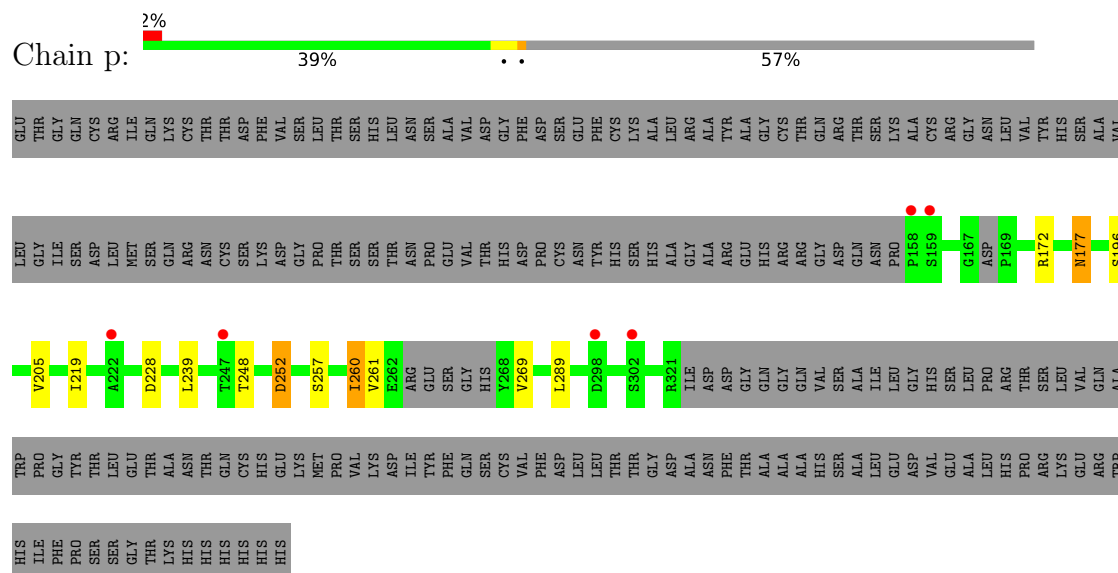
• Molecule 2: RGM domain family member B



• Molecule 2: RGM domain family member B



- Molecule 2: RGM domain family member B



- Molecule 2: RGM domain family member B



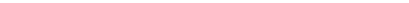
[illegible]

- Molecule 2: RGM domain family member B

Chain T: 99%

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

- Molecule 2: RGM domain family member B

Chain U:  99%

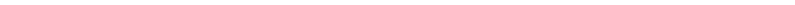
[illegible]

- Molecule 2: RGM domain family member B

Chain V: 1% 1% 99%

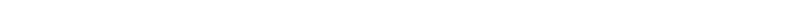
[illegible]

- Molecule 2: RGM domain family member B

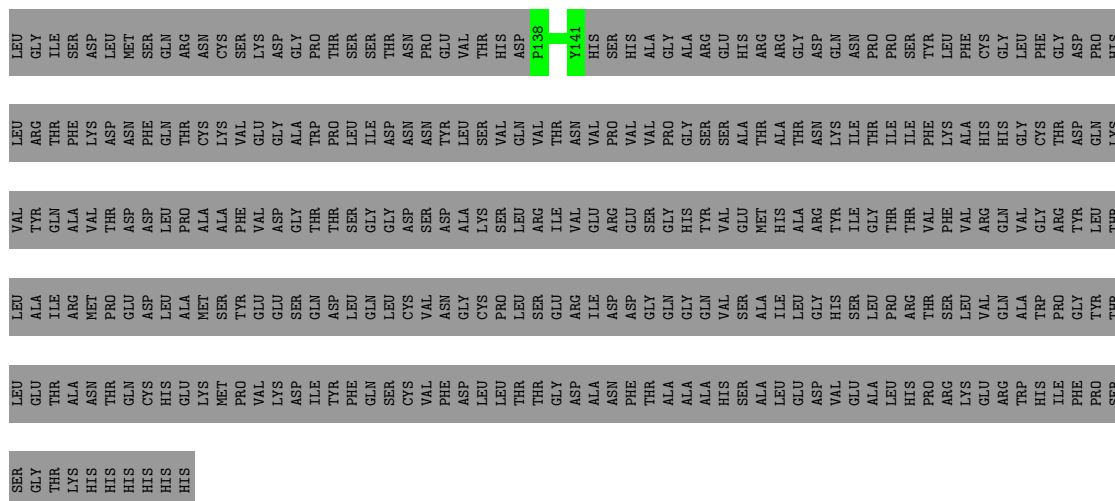
Chain W: 

[illegible]

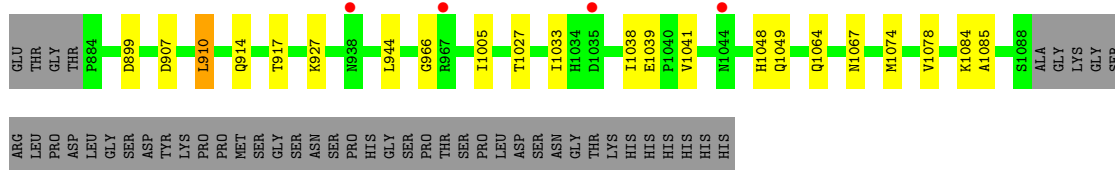
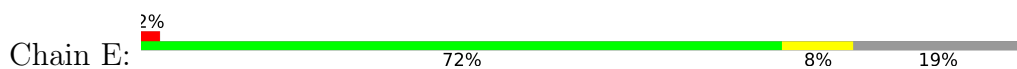
- Molecule 2: RGM domain family member B

Chain X:  99%

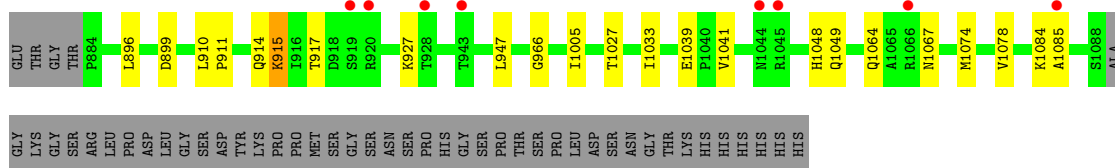
GLU THR GLY GLN CYS ARG ILE GLN LYS CYS THR THR ASP PHE VAL SER SER SER HIS LEU ASN ALA VAL ASP GLY PHE ASP ASP SER SER GLU PHE CYS LYS LEU ARG TYR TYR ALA ALA ALA GLY CYS THR GLN ARG THR THR SER SER LYS ALA CYS ARG ARG GLY ASN LEU VAL TYR THR HIS SER SER ALA VAL



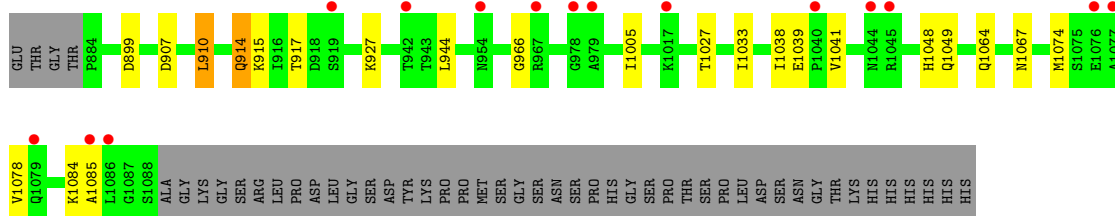
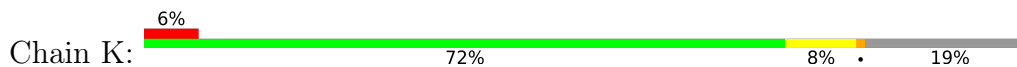
- Molecule 3: Neogenin



- Molecule 3: Neogenin

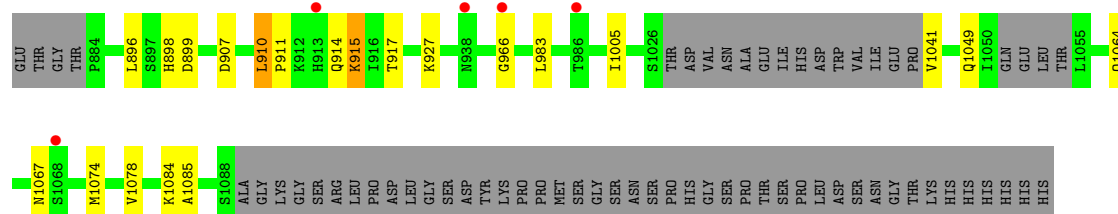


- Molecule 3: Neogenin

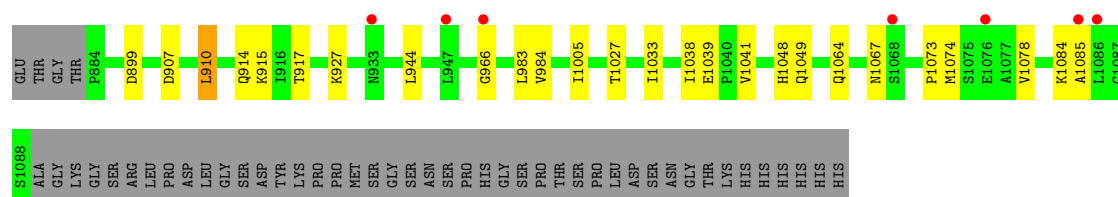


- Molecule 3: Neogenin

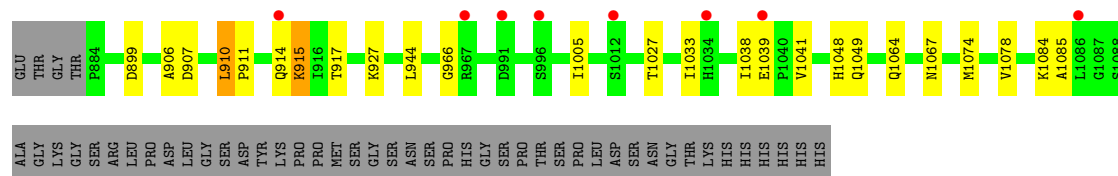




• Molecule 3: Neogenin



• 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.

All (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
2	c	228	ASP	N-CA-C	-6.60	101.02	110.59
2	o	252	ASP	CA-CB-CG	6.51	119.11	112.60
2	c	252	ASP	CA-CB-CG	6.47	119.07	112.60
2	p	252	ASP	CA-CB-CG	6.43	119.03	112.60
2	j	252	ASP	CA-CB-CG	6.37	118.97	112.60
2	d	252	ASP	CA-CB-CG	6.36	118.96	112.60
2	i	252	ASP	CA-CB-CG	6.24	118.84	112.60
3	Q	1027	THR	N-CA-C	-6.02	105.77	113.23
3	K	1027	THR	N-CA-C	-5.99	105.81	113.23
3	F	1027	THR	N-CA-C	-5.98	105.81	113.23
3	E	1027	THR	N-CA-C	-5.96	105.84	113.23
3	R	1027	THR	N-CA-C	-5.90	105.91	113.23
3	L	899	ASP	CA-CB-CG	5.82	118.42	112.60
2	o	205	VAL	N-CA-C	-5.81	104.42	109.19
2	i	205	VAL	N-CA-C	-5.76	104.47	109.19
2	d	205	VAL	N-CA-C	-5.74	104.48	109.19
2	c	205	VAL	N-CA-C	-5.71	104.50	109.19
3	E	899	ASP	CA-CB-CG	5.71	118.31	112.60
3	K	899	ASP	CA-CB-CG	5.68	118.28	112.60
3	R	899	ASP	CA-CB-CG	5.68	118.28	112.60
2	j	205	VAL	N-CA-C	-5.68	104.53	109.19
3	Q	899	ASP	CA-CB-CG	5.61	118.21	112.60
2	p	205	VAL	N-CA-C	-5.55	104.64	109.19
3	F	1033	ILE	N-CA-C	5.54	116.94	110.62
3	F	899	ASP	CA-CB-CG	5.54	118.14	112.60
3	R	1067	ASN	CA-CB-CG	5.52	118.12	112.60
3	R	1033	ILE	N-CA-C	5.51	116.90	110.62
3	K	1033	ILE	N-CA-C	5.50	116.89	110.62
2	p	177	ASN	CA-CB-CG	5.50	118.10	112.60
2	d	177	ASN	CA-CB-CG	5.46	118.06	112.60
3	E	1067	ASN	CA-CB-CG	5.46	118.06	112.60
3	L	1067	ASN	CA-CB-CG	5.45	118.05	112.60
3	E	1033	ILE	N-CA-C	5.44	116.82	110.62
3	Q	1067	ASN	CA-CB-CG	5.44	118.04	112.60
2	c	177	ASN	CA-CB-CG	5.38	117.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1067	ASN	CA-CB-CG	5.37	117.97	112.60
2	o	177	ASN	CA-CB-CG	5.34	117.94	112.60
3	F	1067	ASN	CA-CB-CG	5.33	117.92	112.60
2	i	177	ASN	CA-CB-CG	5.32	117.92	112.60
2	j	177	ASN	CA-CB-CG	5.32	117.92	112.60
3	Q	1033	ILE	N-CA-C	5.31	116.67	110.62
2	o	213	THR	N-CA-C	5.05	116.97	109.25
2	o	180	THR	CB-CA-C	5.03	118.98	110.79
2	c	213	THR	N-CA-C	5.02	116.92	109.25
2	d	213	THR	N-CA-C	5.02	116.92	109.25
2	j	180	THR	CB-CA-C	5.01	118.96	110.79

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	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

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

All (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
1:A:421:PRO:HD3	2:c:162:PHE:CZ	2.10	0.85
1:G:419:ILE:CB	2:i:281:PHE:CZ	2.64	0.80
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:K:910:LEU:HD23	3:K:914:GLN:C	2.13	0.72
2:d:261:VAL:HG23	2:d:270:GLU:HG3	1.73	0.71
2:j:261:VAL:HG23	2:j:270:GLU:HG3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:o:261:VAL:HG23	2:o:270:GLU:HG3	1.73	0.70
2:i:261:VAL:HG23	2:i:270:GLU:HG3	1.73	0.69
2:c:261:VAL:HG23	2:c:270:GLU:HG3	1.73	0.69
3:L:910:LEU:HD23	3:L:914:GLN:CA	2.22	0.69
3:K:910:LEU:HD21	3:K:915:LYS:O	1.94	0.66
1:A:421:PRO:HD3	2:c:162:PHE:HZ	1.61	0.64
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
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
1:A:421:PRO:CD	2:c:162:PHE:CZ	2.87	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:E:910:LEU:HD23	3:E:914:GLN:C	2.33	0.53
3:K:910:LEU:HG	3:K:915:LYS:O	2.08	0.53
2:p:196:SER:HB2	2:p:219:ILE:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:910:LEU:HD23	3:E:914:GLN:HA	1.90	0.53
1:A:487:TYR:CA	2:c:172:ARG:HH11	2.22	0.53
2:d:196:SER:HB2	2:d:219:ILE:HB	1.91	0.52
2:j:196:SER:HB2	2:j:219:ILE:HB	1.91	0.52
1:A:487:TYR:CA	2:c:172:ARG:NH1	2.72	0.52
2:c:196:SER:HB2	2:c:219:ILE:HB	1.91	0.52
1:N:438:ARG:HG3	1:N:440:HIS:CE1	2.44	0.52
2:o:196:SER:HB2	2:o:219:ILE:HB	1.91	0.52
2:i:196:SER:HB2	2:i:219:ILE:HB	1.91	0.51
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
1:A:420:ALA:C	2:c:162:PHE:HE2	2.19	0.51
2:D:119:ARG:HA	4:D:1001:NAG:H82	1.94	0.50
1:A:421:PRO:CD	2:c:162:PHE:HZ	2.25	0.50
2:P:119:ARG:HA	4:P:1001:NAG:H82	1.94	0.50
3:R:910:LEU:CD2	3:R:914:GLN:C	2.79	0.50
3:F:910:LEU:HG	3:F:911:PRO:CD	2.42	0.50
1:A:420:ALA:C	2:c:162:PHE:CE2	2.90	0.49
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
2:J:88:TYR:O	2:J:92:THR:HG23	2.13	0.49
3:Q:910:LEU:CD2	3:Q:914:GLN:C	2.80	0.49
2:o:248:THR:HA	2:o:260:ILE:HD12	1.95	0.49
2:i:248:THR:HA	2:i:260:ILE:HD12	1.95	0.48
2:c:248:THR:HA	2:c:260:ILE:HD12	1.95	0.48
2:O:88:TYR:O	2:O:92:THR:HG23	2.13	0.48
2:j:248:THR:HA	2:j:260:ILE:HD12	1.95	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
2:d:248:THR:HA	2:d:260:ILE:HD12	1.95	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
1:G:419:ILE:CB	2:i:281:PHE:CE2	2.98	0.47
3:L:910:LEU:CD2	3:L:914:GLN:C	2.81	0.47
2:p:248:THR:HA	2:p:260:ILE:HD12	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ARG:HG2	1:B:441:LEU:HG	1.98	0.46
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: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
2:d:239:LEU:HD11	2:d:289:LEU:HD22	2.00	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
2:i:239:LEU:HD11	2:i:289:LEU:HD22	2.00	0.44
2:j:239:LEU:HD11	2:j:289:LEU:HD22	2.00	0.44
1:H:417:TRP:CZ3	2:J:101:GLY:HA2	2.52	0.44
2:o:239:LEU:HD11	2:o:289:LEU:HD22	2.00	0.44
2:D:116:MET:HE2	2:D:116:MET:HB3	1.91	0.43
1:G:441:LEU:HD13	1:G:500:CYS:SG	2.58	0.43
2:p:239:LEU:HD11	2:p:289:LEU:HD22	2.00	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:c:239:LEU:HD11	2:c:289:LEU:HD22	1.99	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
3:R:911:PRO:HB2	3:R:915:LYS:HZ3	1.83	0.42
2:I:116:MET:HE2	2:I:116:MET:HB3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:c:161:LEU:HD11	2:c:297:GLU:HG3	2.03	0.41
1:A:487:TYR:O	2:c:178:PHE:HZ	2.04	0.41
1:G:396:LEU:HD22	2:J:71:ASN:HD21	1.86	0.41
3:K:910:LEU:CD2	3:K:914:GLN:C	2.90	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
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
2:d:161:LEU:HD11	2:d:297:GLU:HG3	2.04	0.40
1:B:417:TRP:CZ3	2:D:101:GLY:HA2	2.57	0.40
2:o:161:LEU:HD11	2:o:297:GLU:HG3	2.03	0.40
1:A:421:PRO:HA	2:c:294:ARG:HD2	2.03	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

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

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	966	GLY
3	F	966	GLY

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Mol	Chain	Res	Type
3	K	966	GLY
3	L	966	GLY
3	Q	966	GLY
3	R	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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	438	ARG
1	B	438	ARG
2	D	74	VAL
3	E	910	LEU
3	E	917	THR
3	E	927	LYS
3	E	1038	ILE
3	E	1041	VAL
3	E	1078	VAL
3	F	915	LYS
3	F	917	THR
3	F	927	LYS
3	F	1041	VAL
3	F	1078	VAL
1	G	438	ARG
1	H	438	ARG
3	K	910	LEU
3	K	914	GLN
3	K	917	THR
3	K	927	LYS
3	K	1038	ILE
3	K	1041	VAL
3	K	1078	VAL

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Mol	Chain	Res	Type
3	L	910	LEU
3	L	915	LYS
3	L	917	THR
3	L	927	LYS
3	L	1041	VAL
3	L	1078	VAL
1	M	438	ARG
1	N	438	ARG
2	P	74	VAL
3	Q	910	LEU
3	Q	915	LYS
3	Q	917	THR
3	Q	927	LYS
3	Q	1038	ILE
3	Q	1041	VAL
3	Q	1078	VAL
3	R	910	LEU
3	R	915	LYS
3	R	917	THR
3	R	927	LYS
3	R	1038	ILE
3	R	1041	VAL
3	R	1078	VAL
2	c	172	ARG
2	c	177	ASN
2	c	252	ASP
2	c	257	SER
2	c	260	ILE
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	260	ILE
2	d	261	VAL
2	d	269	VAL
2	i	177	ASN
2	i	252	ASP
2	i	257	SER
2	i	260	ILE
2	i	261	VAL

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Mol	Chain	Res	Type
2	i	269	VAL
2	j	177	ASN
2	j	252	ASP
2	j	257	SER
2	j	260	ILE
2	j	261	VAL
2	j	269	VAL
2	o	177	ASN
2	o	252	ASP
2	o	257	SER
2	o	260	ILE
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	260	ILE
2	p	261	VAL
2	p	269	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	440	HIS
2	C	69	HIS
1	G	440	HIS
1	N	440	HIS
3	Q	898	HIS
3	Q	977	HIS
2	c	214	ASN
2	d	214	ASN
2	i	214	ASN
2	j	214	ASN
2	j	223	HIS
2	o	214	ASN
2	p	214	ASN
2	p	223	HIS

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.

All (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
4	R	2001	NAG	C1-O5-C5	2.64	115.73	112.19

There are no chirality outliers.

There are no torsion outliers.

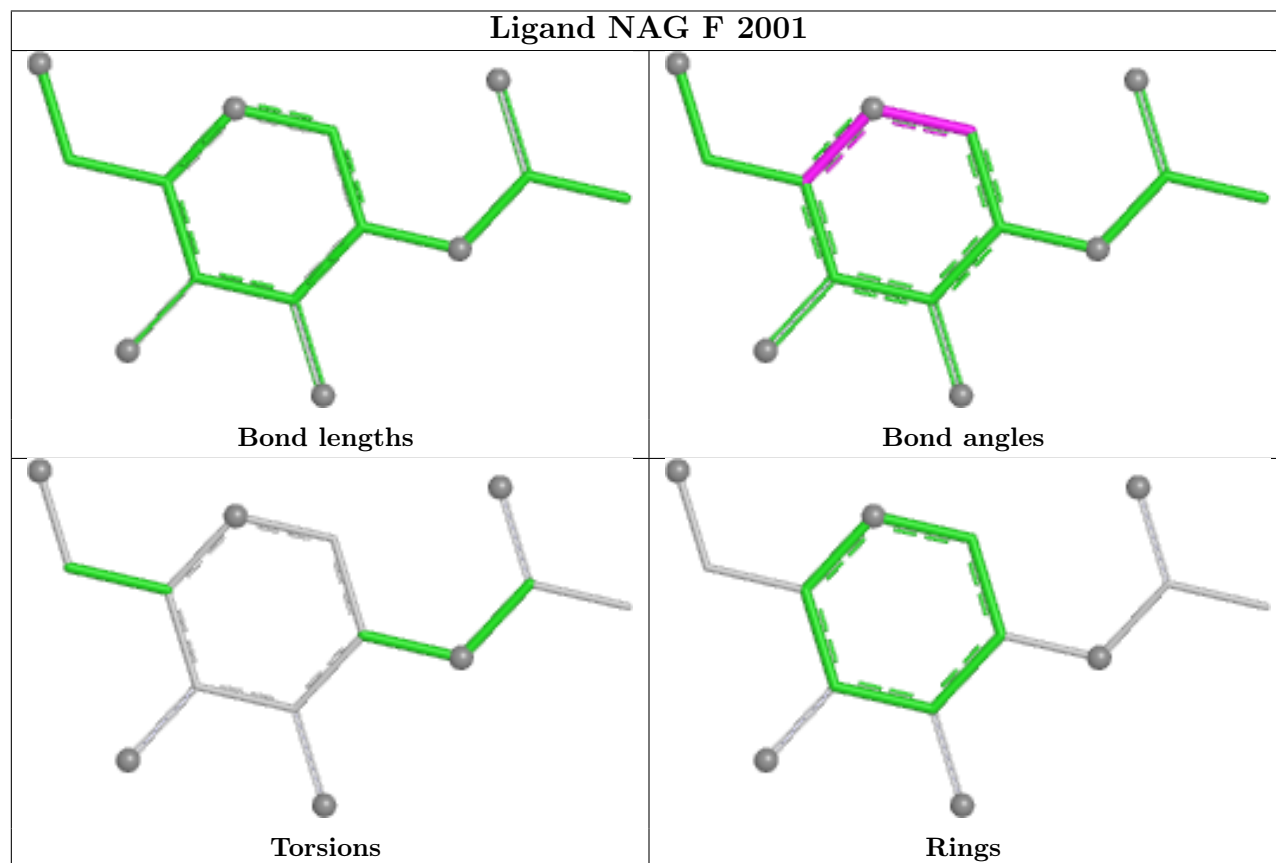
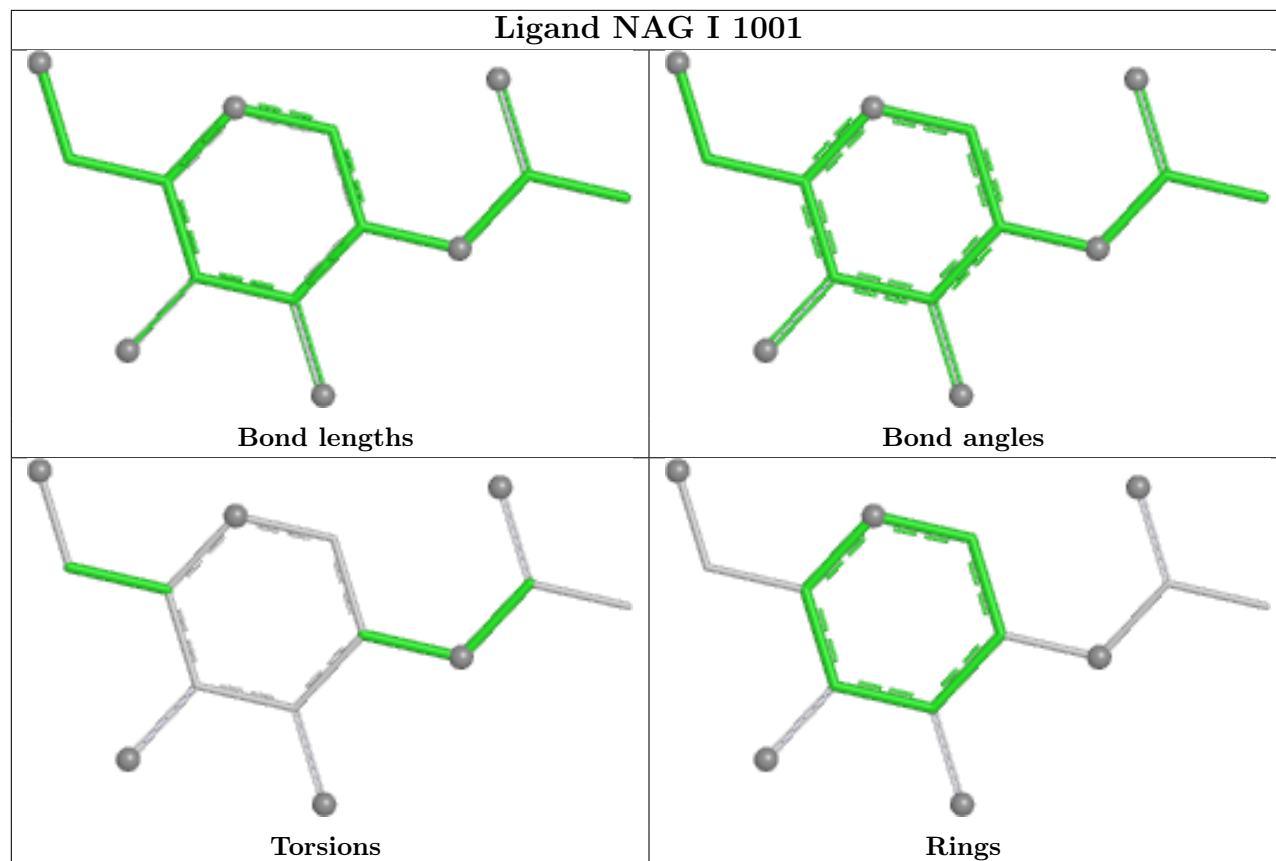
There are no ring outliers.

3 monomers are involved in 3 short contacts:

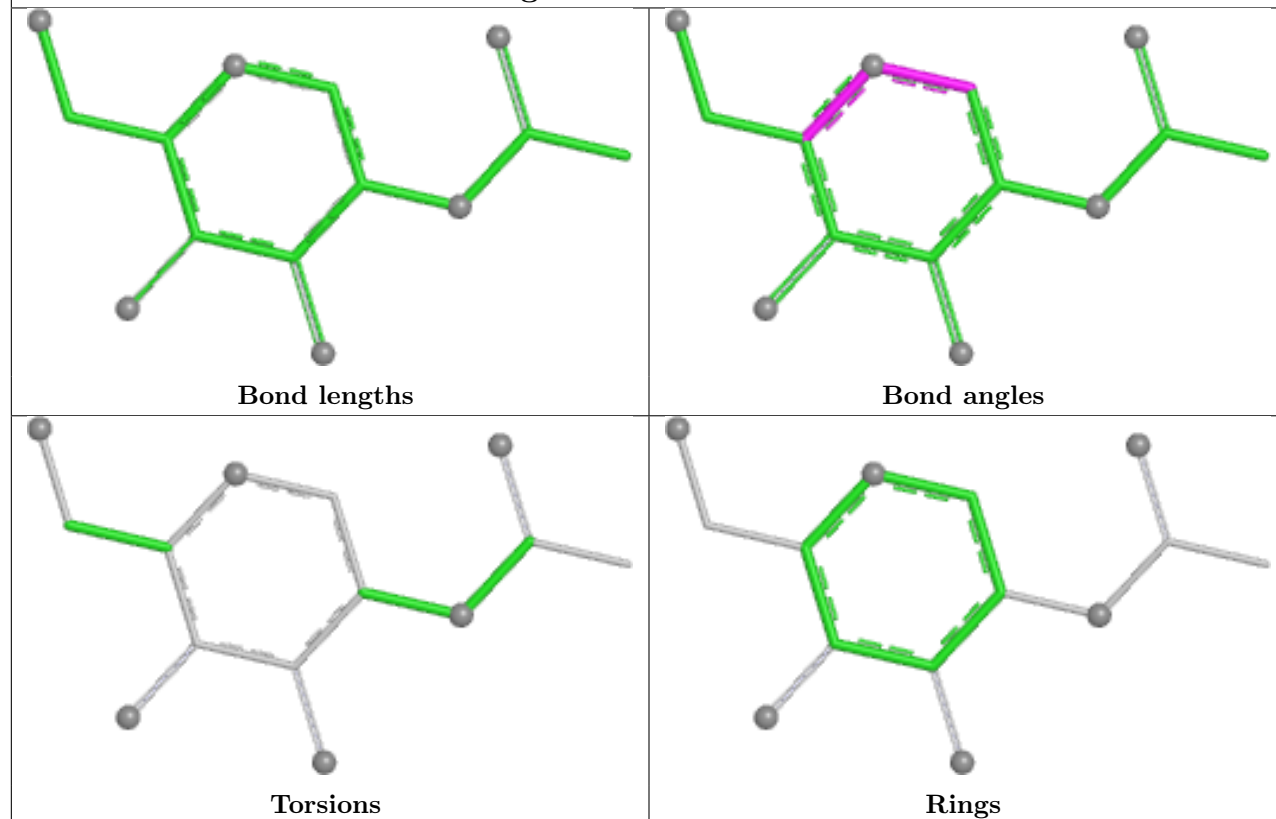
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1001	NAG	1	0
4	P	1001	NAG	1	0
4	D	1001	NAG	1	0

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

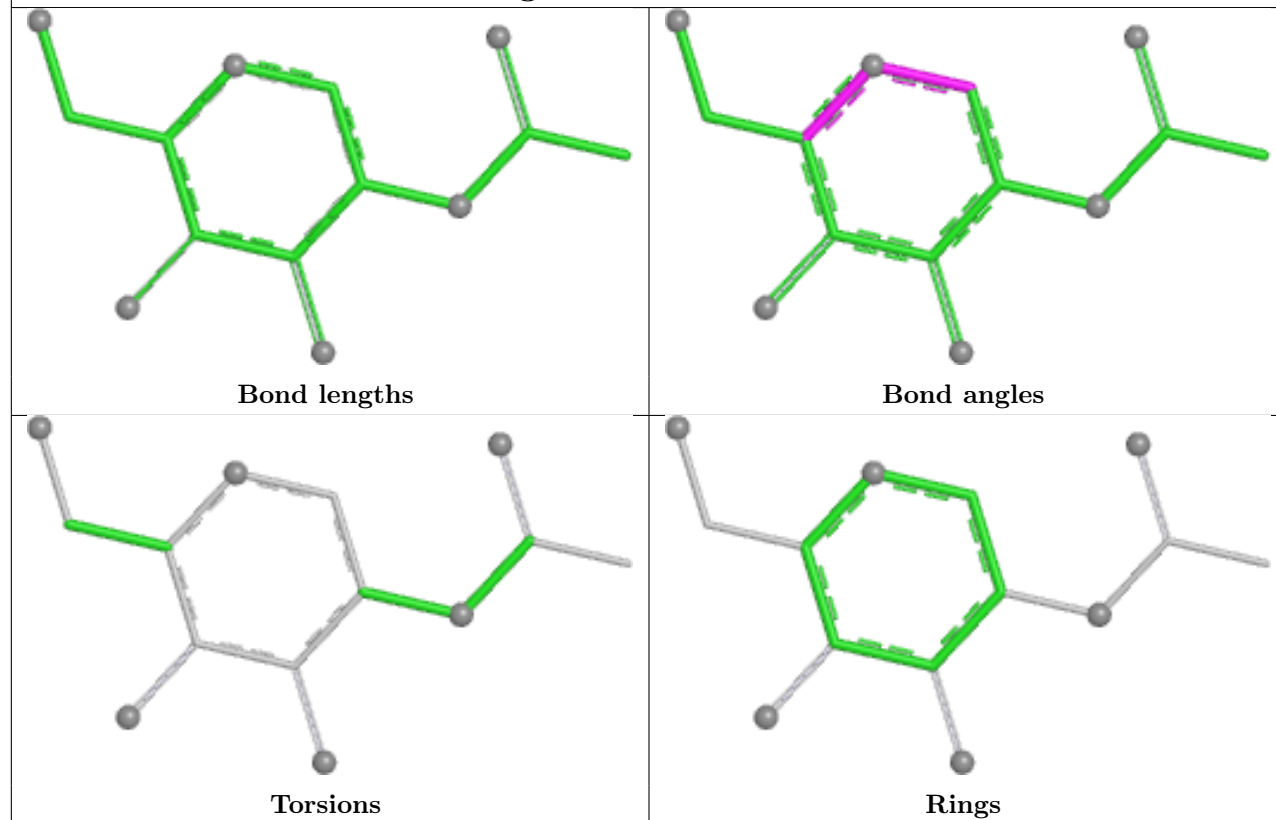
equivalents in the CSD to analyse the geometry.



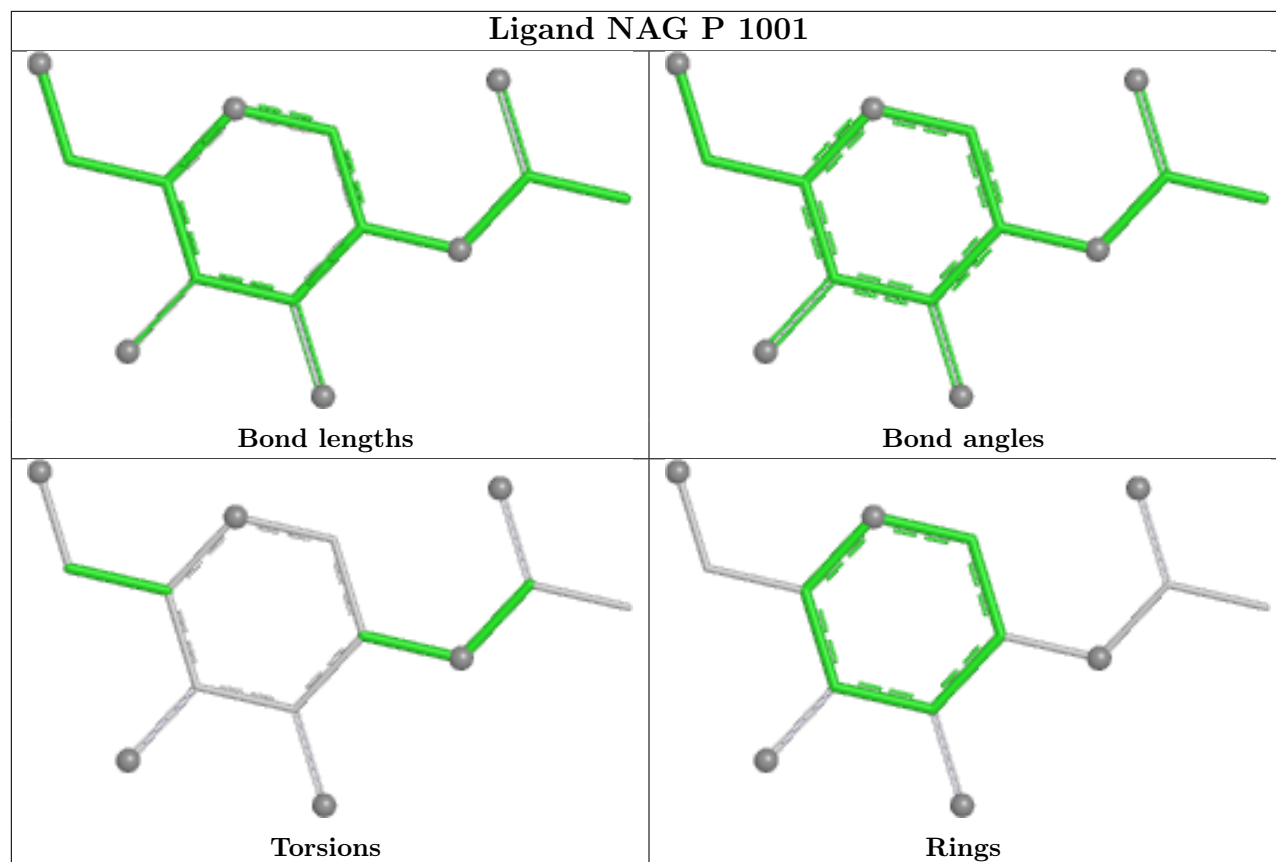
Ligand NAG E 2001



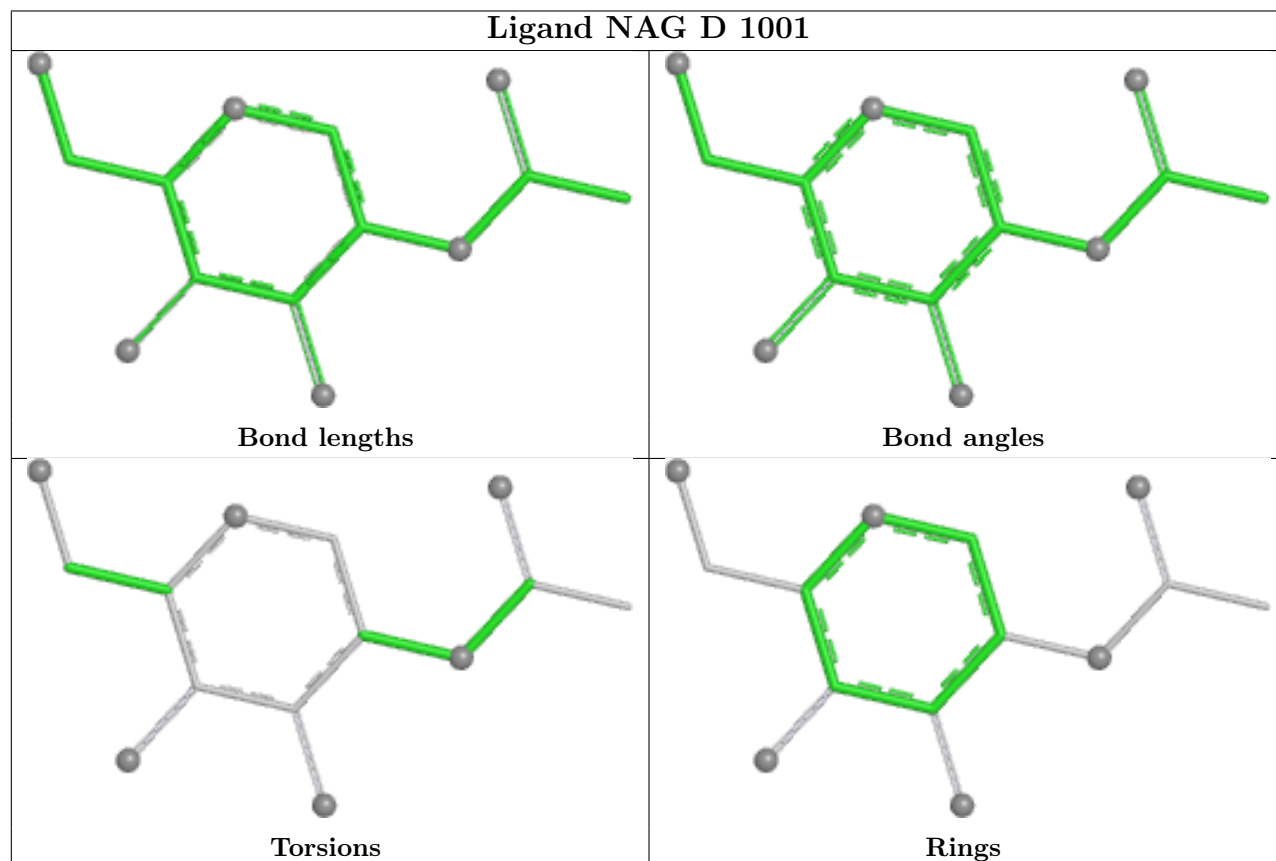
Ligand NAG R 2001



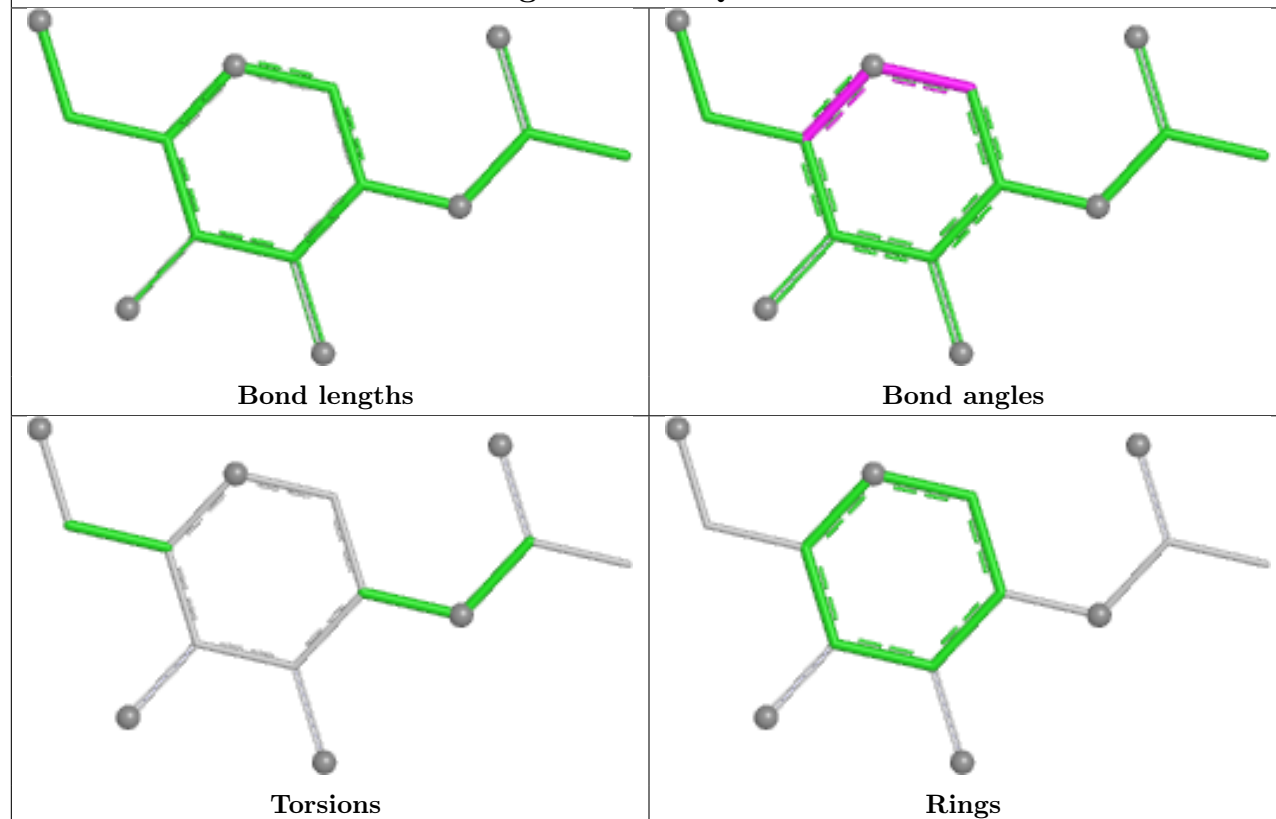
Ligand NAG P 1001



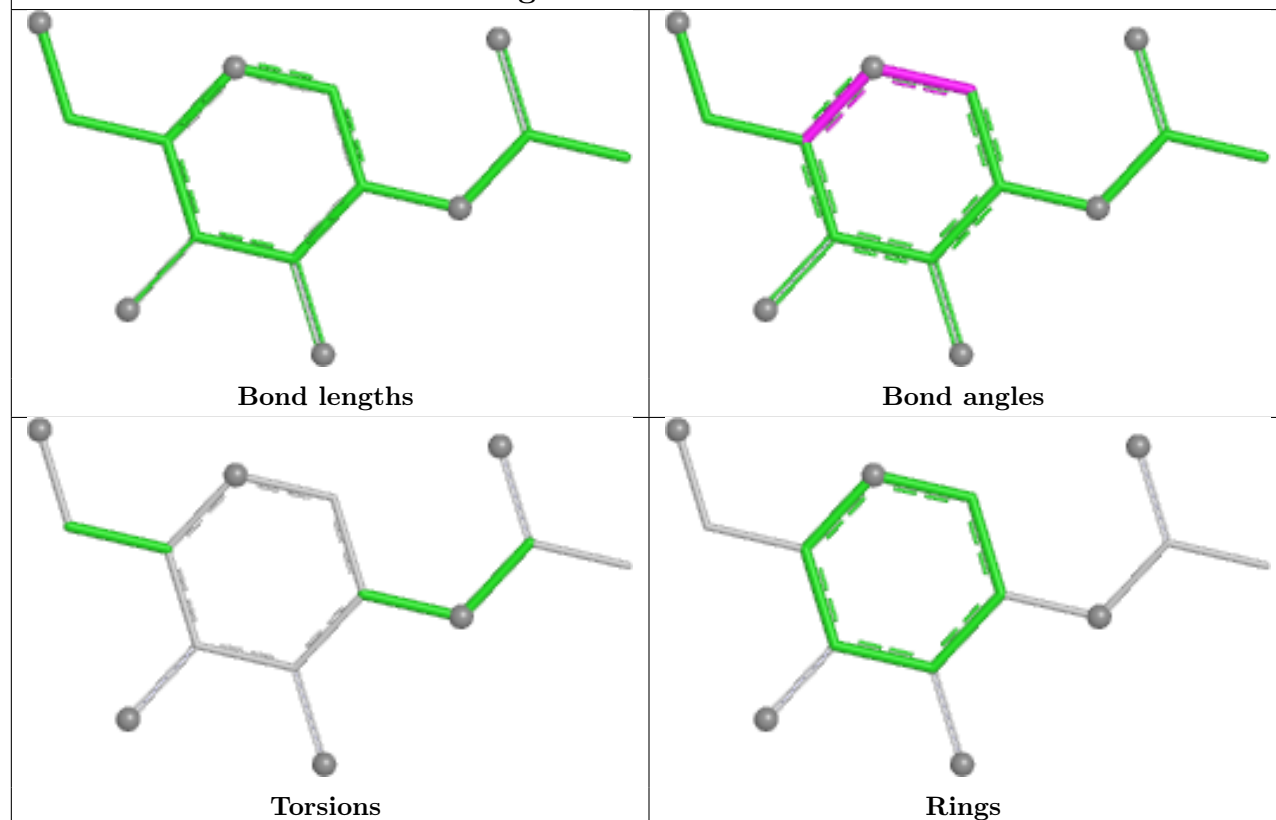
Ligand NAG D 1001

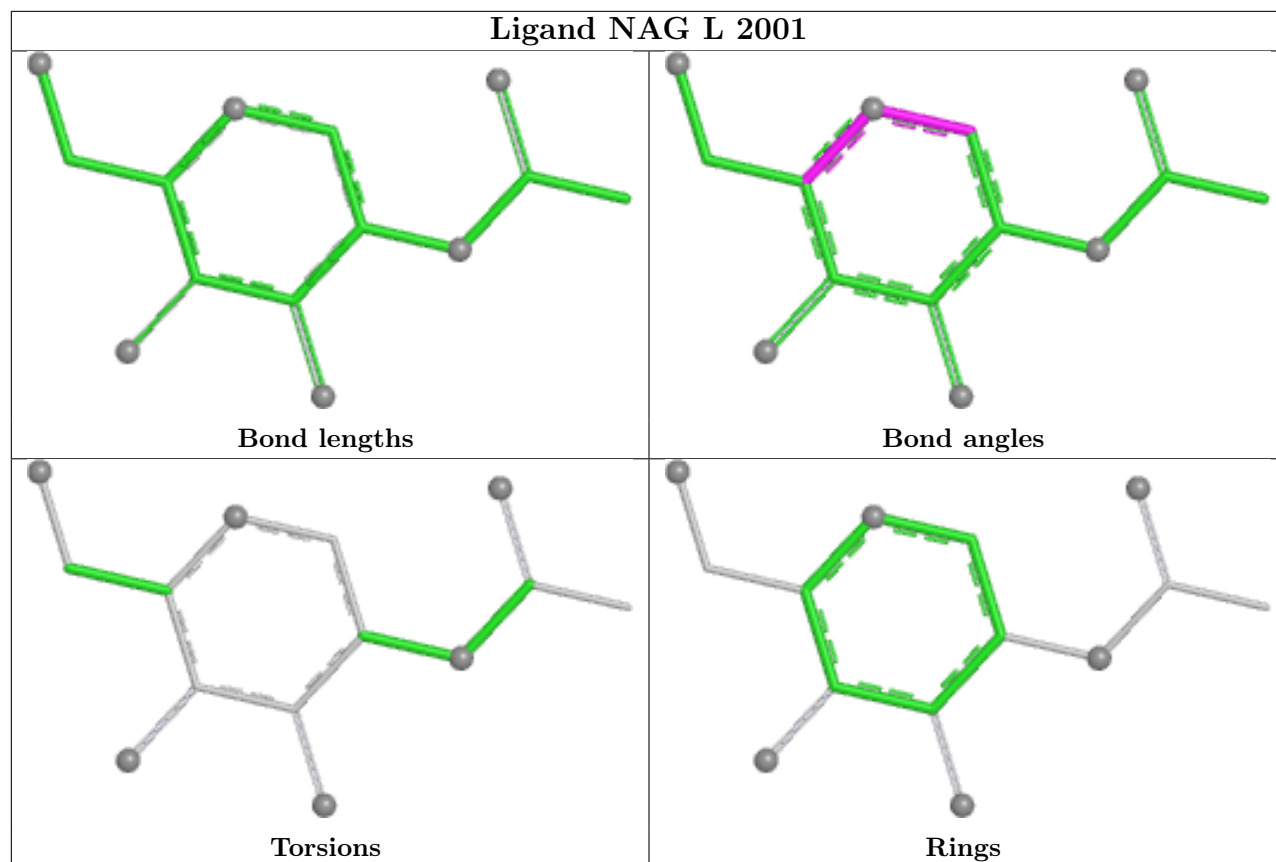


Ligand NAG Q 2001



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

All (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
3	L	913	HIS	4.6
2	O	78	ASP	4.2
2	J	113	SER	4.0
2	i	249	SER	3.7
3	F	1044	ASN	3.6
2	o	158	PRO	3.6
2	d	158	PRO	3.6
2	C	65	SER	3.4
3	E	1044	ASN	3.3
2	p	158	PRO	3.3
3	Q	1086	LEU	3.2
1	M	469	THR	3.2
3	K	1079	GLN	3.2
2	o	275	TYR	3.2
1	H	500	CYS	3.2
3	R	1086	LEU	3.2
2	D	108	ALA	3.2
3	K	979	ALA	3.1
2	d	165	LEU	3.1
2	P	93	GLN	3.1
2	j	159	SER	3.1
2	I	85	LEU	3.1
2	I	87	ALA	3.1
2	c	297	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	O	81	PHE	3.0
3	F	919	SER	2.9
2	j	158	PRO	2.9
3	K	919	SER	2.9
2	j	305	GLU	2.9
2	P	80	GLU	2.9
3	K	1044	ASN	2.9
2	I	95	THR	2.8
3	K	1076	GLU	2.8
2	P	75	ASP	2.8
2	i	297	GLU	2.8
2	p	247	THR	2.8
3	K	967	ARG	2.8
2	o	276	ILE	2.7
1	B	500	CYS	2.7
1	H	469	THR	2.7
2	i	312	CYS	2.7
2	p	159	SER	2.7
2	c	176	ASP	2.7
3	K	978	GLY	2.7
1	A	470	ARG	2.7
3	F	943	THR	2.7
1	B	475	SER	2.7
2	j	193	ASN	2.7
3	Q	1076	GLU	2.6
2	p	298	ASP	2.6
2	o	262	GLU	2.6
2	i	229	GLN	2.6
2	i	319	SER	2.6
3	R	991	ASP	2.6
3	F	1085	ALA	2.6
2	I	52	GLY	2.6
2	i	262	GLU	2.6
2	C	72	SER	2.5
2	i	245	ASP	2.5
3	K	1077	ALA	2.5
1	B	501	ARG	2.5
2	j	306	SER	2.5
1	A	465	CYS	2.5
2	i	222	ALA	2.5
2	I	96	SER	2.5
2	D	93	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
2	d	253	SER	2.4
2	i	268	TYR	2.4
3	K	942	THR	2.4
3	Q	1085	ALA	2.4
2	O	76	GLY	2.4
1	B	434	GLU	2.4
2	d	262	GLU	2.4
3	F	928	THR	2.4
2	P	73	ALA	2.4
2	c	158	PRO	2.4
3	L	986	THR	2.4
2	j	259	ARG	2.4
3	Q	947	LEU	2.4
3	E	1035	ASP	2.3
2	d	229	GLN	2.3
2	J	116	MET	2.3
3	L	966	GLY	2.3
2	I	84	ALA	2.3
1	B	433	CYS	2.3
2	I	93	GLN	2.3
2	j	192	ASN	2.3
3	L	938	ASN	2.3
2	i	247	THR	2.3
2	d	269	VAL	2.3
1	G	442	GLU	2.3
3	K	954	ASN	2.3
1	N	487	TYR	2.2
2	W	138	PRO	2.2
1	M	470	ARG	2.2
2	O	77	PHE	2.2
2	I	54	CYS	2.2
3	K	1017	LYS	2.2
2	J	64	VAL	2.2
3	Q	1068	SER	2.2
1	G	501	ARG	2.2
2	P	113	SER	2.2
2	p	302	SER	2.2
3	R	1034	HIS	2.2
2	J	124	ASP	2.2
3	F	1066	ARG	2.2
2	V	140	ASN	2.2
3	K	1040	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	N	475	SER	2.2
2	W	141	TYR	2.2
1	G	463	PRO	2.2
3	L	1068	SER	2.2
2	J	114	ASP	2.1
2	P	126	PRO	2.1
2	d	298	ASP	2.1
3	K	1085	ALA	2.1
3	Q	933	ASN	2.1
2	V	138	PRO	2.1
2	j	258	LEU	2.1
3	R	967	ARG	2.1
3	R	914	GLN	2.1
2	J	73	ALA	2.1
2	I	86	ARG	2.1
2	P	69	HIS	2.1
3	R	1012	SER	2.1
3	R	1039	GLU	2.1
2	o	194	TYR	2.1
3	E	938	ASN	2.1
2	j	242	ALA	2.1
1	H	470	ARG	2.1
3	K	1045	ARG	2.1
3	Q	966	GLY	2.1
3	R	996	SER	2.1
1	H	442	GLU	2.0
2	j	209	SER	2.0
3	F	920	ARG	2.0
2	i	194	TYR	2.0
2	C	124	ASP	2.0
2	j	261	VAL	2.0
1	G	470	ARG	2.0
3	F	1045	ARG	2.0
2	J	72	SER	2.0
2	o	159	SER	2.0
2	i	160	TYR	2.0
2	I	127	THR	2.0
3	E	967	ARG	2.0

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

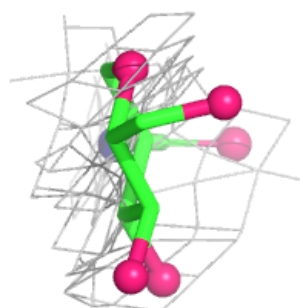
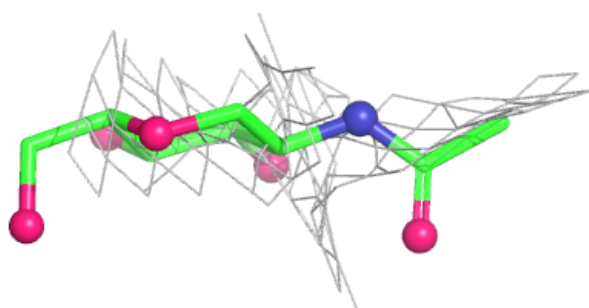
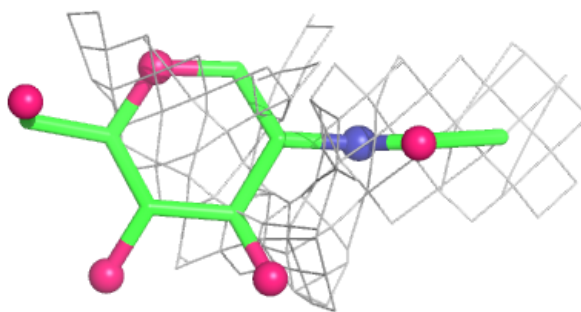
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	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
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

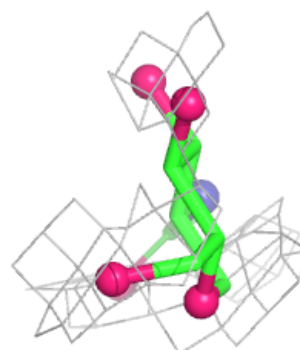
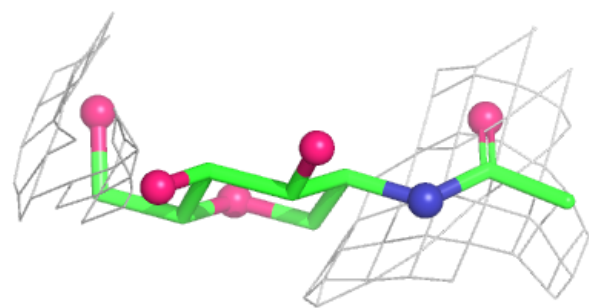
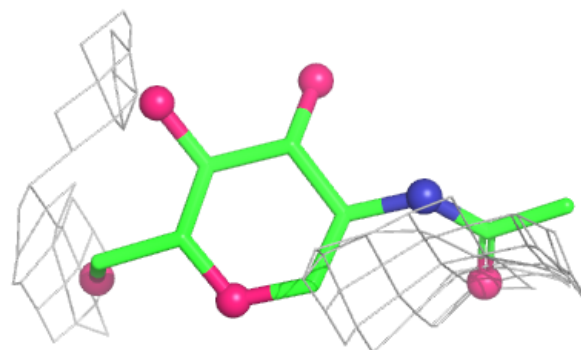
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

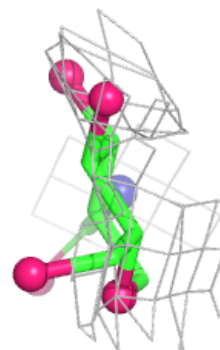
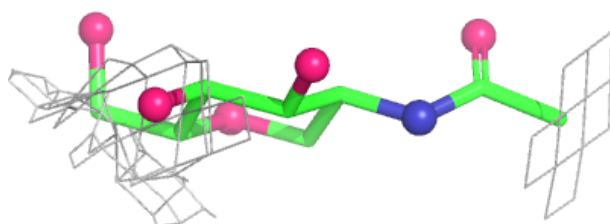
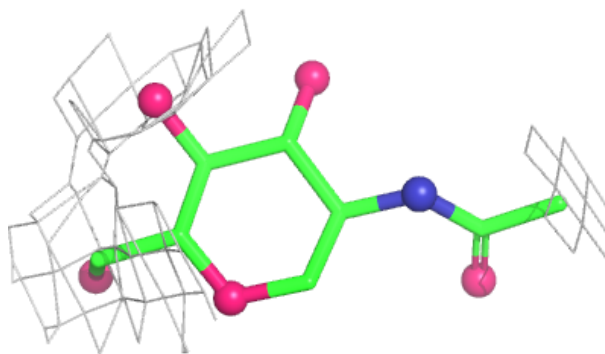
**Electron density around NAG P 1001:**

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

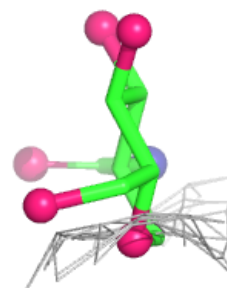
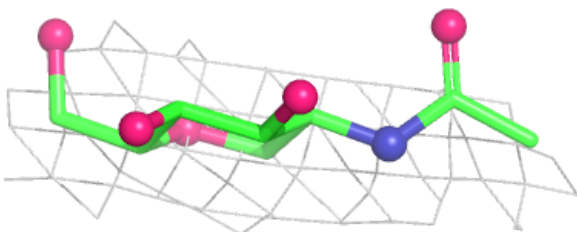
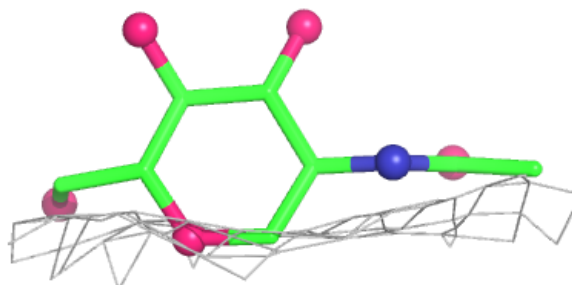


Electron density around NAG I 1001:

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

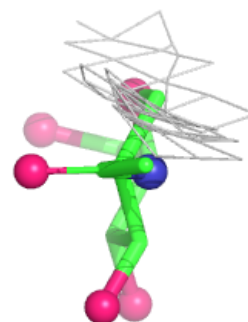
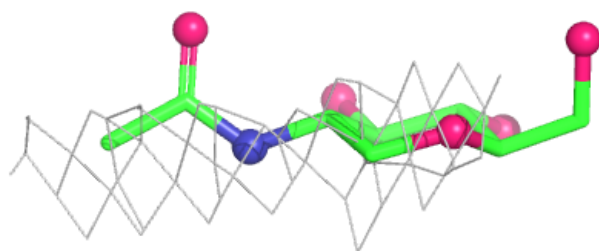
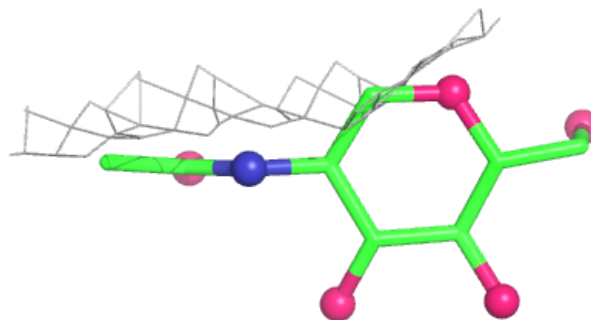
**Electron density around NAG L 2001:**

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

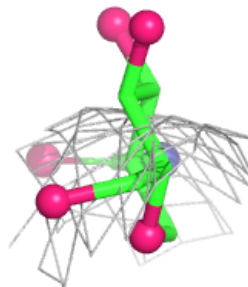
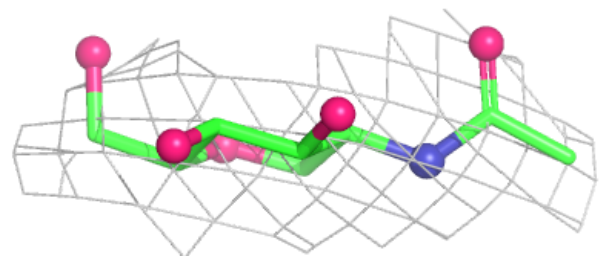
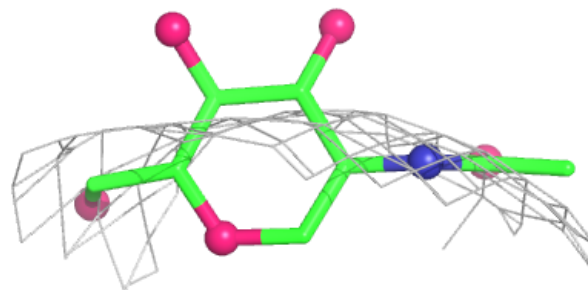


Electron density around NAG R 2001:

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

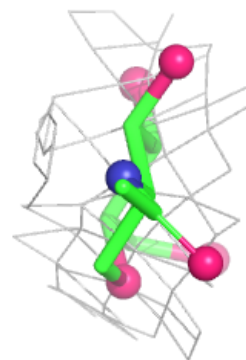
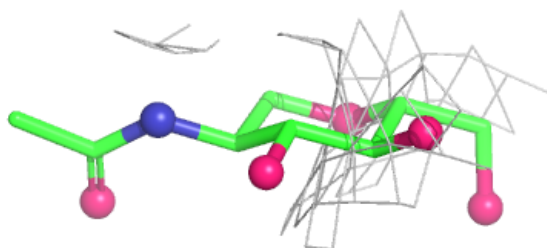
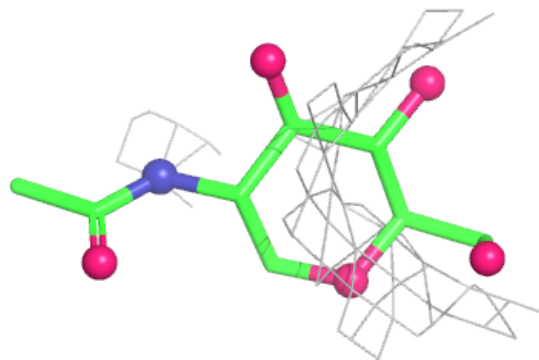
**Electron density around NAG Q 2001:**

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

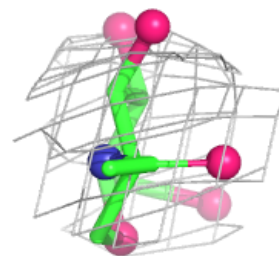
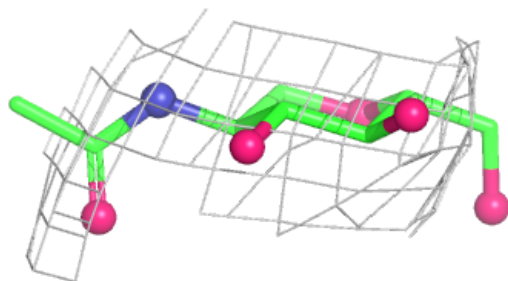
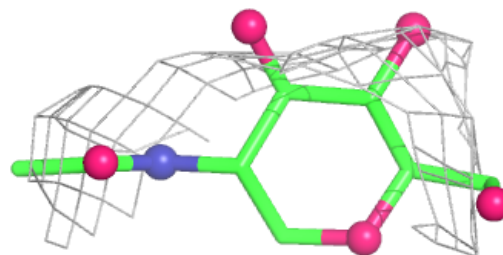


Electron density around NAG D 1001:

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

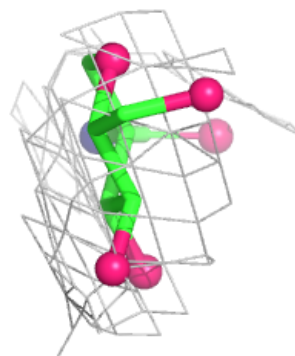
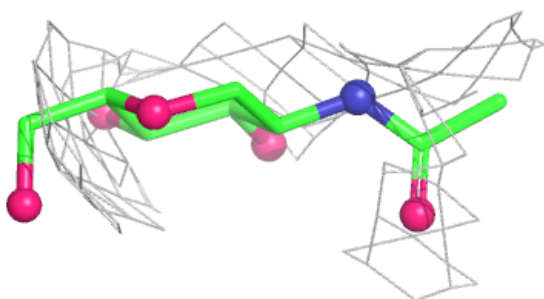
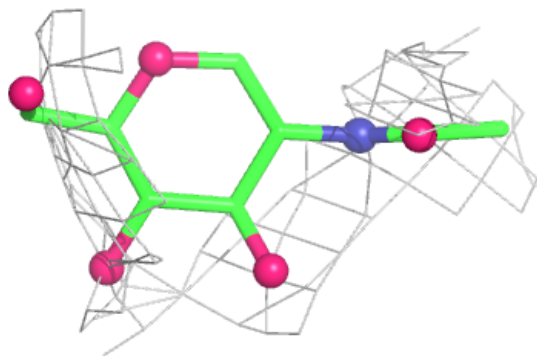
**Electron density around NAG E 2001:**

$2mF_o - DF_c$ (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.