Full wwPDB X-ray Structure Validation Report (i)

Apr 6, 2020 – 02:40 PM EDT

PDB ID	:	6WGL
Title	:	Dupilumab-fab and IL4R domain complex
Deposited on	:	2020-04-05
Resolution	:	2.82 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

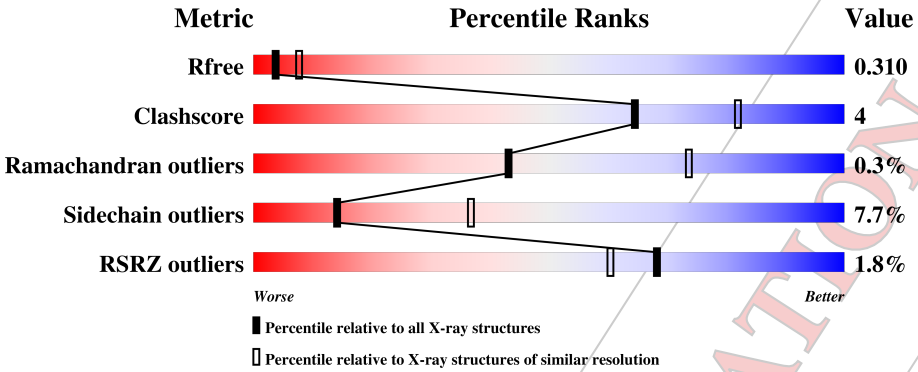
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.10.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.10.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

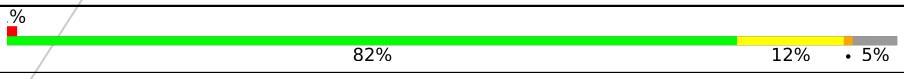
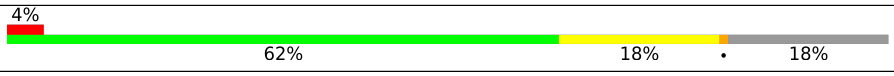
The reported resolution of this entry is 2.82 Å.

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}	111664	3177 (2.84-2.80)
Clashscore	122126	3606 (2.84-2.80)
Ramachandran outliers	120053	3547 (2.84-2.80)
Sidechain outliers	120020	3549 (2.84-2.80)
RSRZ outliers	108989	3108 (2.84-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	234	
2	B	217	
3	C	218	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4743 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 Dupilumab Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	222	1632	1024	274	326	8	0	1	0

- Molecule 2 is a protein called Dupilumab Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	216	1632	1026	266	334	6	0	1	0

- Molecule 3 is a protein called Interleukin-4 receptor subunit alpha.

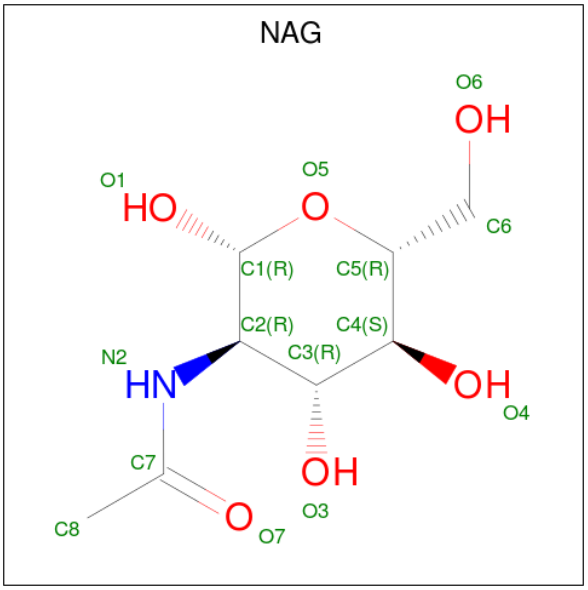
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	178	1383	889	224	260	10	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	182	LEU	CYS	conflict	UNP P24394
C	208	GLY	-	expression tag	UNP P24394
C	209	GLY	-	expression tag	UNP P24394
C	210	GLY	-	expression tag	UNP P24394
C	211	GLY	-	expression tag	UNP P24394
C	212	SER	-	expression tag	UNP P24394
C	213	HIS	-	expression tag	UNP P24394
C	214	HIS	-	expression tag	UNP P24394
C	215	HIS	-	expression tag	UNP P24394
C	216	HIS	-	expression tag	UNP P24394
C	217	HIS	-	expression tag	UNP P24394
C	218	HIS	-	expression tag	UNP P24394

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$)

(labeled as "Ligand of Interest" by author).



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

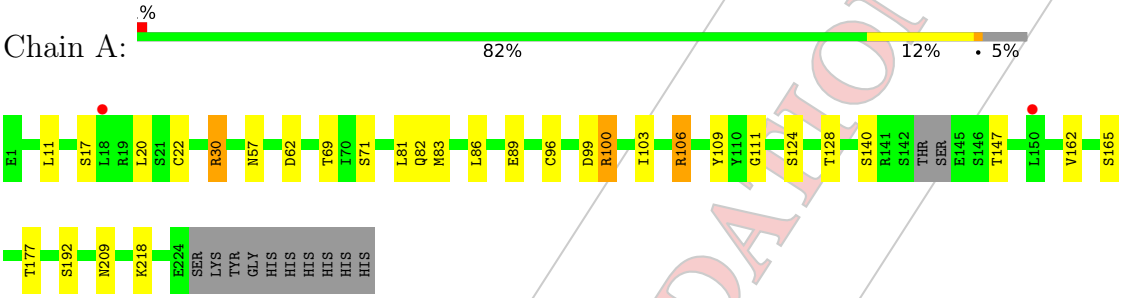
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	6	Total O 6 6	0	0
5	B	11	Total O 11 11	0	0
5	C	9	Total O 9 9	0	0

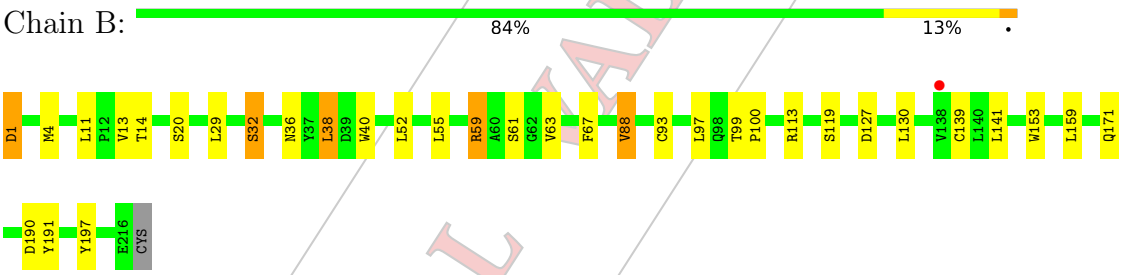
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

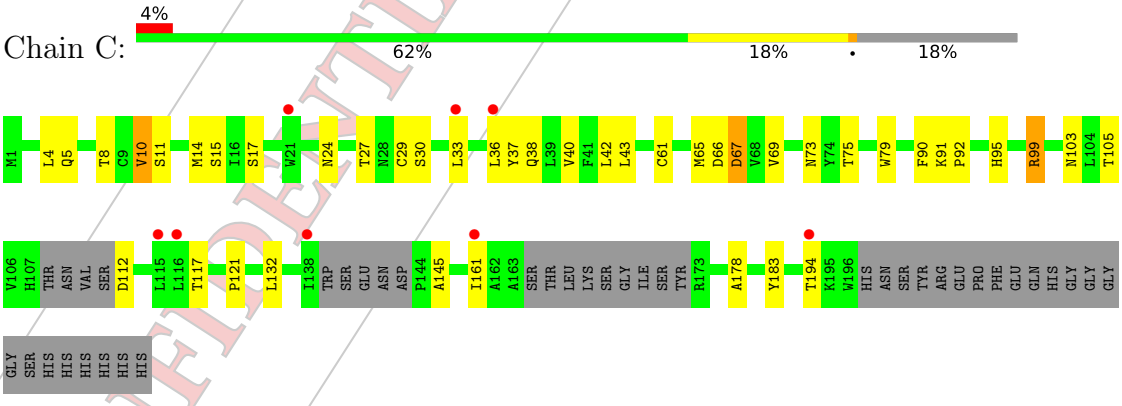
• Molecule 1: Dupilumab Fab heavy chain



• Molecule 2: Dupilumab Fab light chain



• Molecule 3: Interleukin-4 receptor subunit alpha



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	73.49Å 73.49Å 412.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.82 103.11 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.82) 99.9 (103.11-2.82)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.245 , 0.304 0.248 , 0.310	Depositor DCC
R_{free} test set	1423 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	75.7	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 70.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4743	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.32	0/1671	0.69	0/2279
2	B	0.32	0/1670	0.69	0/2273
3	C	0.30	0/1422	0.70	2/1950 (0.1%)
All	All	0.31	0/4763	0.69	2/6502 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	2
3	C	0	1
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	112	ASP	CB-CG-OD2	6.92	124.52	118.30
3	C	67	ASP	CB-CA-C	5.19	120.78	110.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ARG	Sidechain
1	A	106	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	30	ARG	Sidechain
2	B	113	ARG	Sidechain
2	B	59	ARG	Sidechain
3	C	99	ARG	Sidechain

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	1632	0	1555	12	0
2	B	1632	0	1553	14	0
3	C	1383	0	1299	17	0
4	C	70	0	63	1	0
5	A	6	0	0	0	0
5	B	11	0	0	0	1
5	C	9	0	0	0	0
All	All	4743	0	4470	38	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (38) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:CYS:HG	1:A:96:CYS:HG	1.03	0.83
1:A:57:ASN:HD21	3:C:38:GLN:HE22	1.40	0.69
1:A:83:MET:HB3	1:A:86:LEU:HD21	1.73	0.69
3:C:132:LEU:HD22	3:C:178:ALA:HB1	1.74	0.67
2:B:32:SER:HB2	3:C:69:VAL:HG21	1.76	0.66
1:A:69:THR:HB	1:A:82:GLN:HB3	1.78	0.66
3:C:14:MET:O	3:C:67:ASP:HA	2.00	0.61
2:B:59:ARG:NH1	2:B:67:PHE:O	2.36	0.58
2:B:127:ASP:HA	2:B:130:LEU:HD12	1.87	0.56
2:B:52:LEU:HA	2:B:63:VAL:HG21	1.92	0.52
1:A:11:LEU:HD11	1:A:124:SER:HB3	1.92	0.51
2:B:99:THR:HG23	3:C:42:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:10:VAL:HG12	3:C:95:HIS:HB3	1.93	0.50
3:C:183:TYR:HB2	4:C:303:NAG:H83	1.93	0.50
2:B:139:CYS:HB2	2:B:153:TRP:CZ2	2.46	0.49
1:A:109:TYR:CZ	1:A:111:GLY:HA2	2.47	0.49
2:B:40:TRP:CZ3	2:B:93:CYS:HB3	2.49	0.47
2:B:88:VAL:HG21	2:B:171:GLN:HB3	1.96	0.47
2:B:1:ASP:HB3	2:B:100:PRO:HD2	1.97	0.46
1:A:106:ARG:NH1	3:C:67:ASP:O	2.48	0.46
2:B:141:LEU:N	2:B:141:LEU:HD12	2.30	0.46
2:B:4:MET:CE	2:B:38:LEU:HD21	2.45	0.46
1:A:100:ARG:HD2	3:C:43:LEU:HB2	1.98	0.46
3:C:37:TYR:HA	3:C:75:THR:O	2.16	0.46
3:C:11:SER:HB3	3:C:17:SER:OG	2.17	0.45
3:C:36:LEU:HD12	3:C:79:TRP:CD1	2.52	0.45
3:C:65:MET:HE1	3:C:92:PRO:HG3	1.98	0.44
3:C:73:ASN:HB2	3:C:91:LYS:HG2	1.99	0.43
3:C:11:SER:HA	3:C:17:SER:HA	2.00	0.43
2:B:191:TYR:HA	2:B:197:TYR:OH	2.18	0.43
1:A:20:LEU:HD12	1:A:81:LEU:HD23	2.01	0.42
3:C:29:CYS:HA	3:C:33:LEU:HD12	2.01	0.42
2:B:36:ASN:O	2:B:55:LEU:HD23	2.18	0.42
1:A:99:ASP:OD1	1:A:100:ARG:N	2.53	0.42
3:C:99:ARG:HD2	3:C:121:PRO:HB2	2.02	0.41
2:B:29:LEU:HA	2:B:97:LEU:HD22	2.03	0.41
1:A:165:SER:HB3	1:A:209:ASN:HB2	2.03	0.41
1:A:177:THR:HG23	1:A:192:SER:HB2	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:304:HOH:O	5:B:310:HOH:O[7_645]	2.12	0.08

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	219/234 (94%)	210 (96%)	9 (4%)	0	100	100
2	B	215/217 (99%)	200 (93%)	15 (7%)	0	100	100
3	C	170/218 (78%)	153 (90%)	15 (9%)	2 (1%)	14	40
All	All	604/669 (90%)	563 (93%)	39 (6%)	2 (0%)	43	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	145	ALA
3	C	40	VAL

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	177/198 (89%)	166 (94%)	11 (6%)	20	49
2	B	181/191 (95%)	169 (93%)	12 (7%)	18	45
3	C	149/194 (77%)	133 (89%)	16 (11%)	7	21
All	All	507/583 (87%)	468 (92%)	39 (8%)	14	37

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	30	ARG
1	A	62	ASP
1	A	71	SER
1	A	89	GLU
1	A	103	ILE
1	A	128	THR
1	A	140	SER

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Mol	Chain	Res	Type
1	A	147	THR
1	A	162	VAL
1	A	218	LYS
2	B	1	ASP
2	B	11	LEU
2	B	13	VAL
2	B	14	THR
2	B	20	SER
2	B	32	SER
2	B	38	LEU
2	B	61	SER
2	B	88	VAL
2	B	119	SER
2	B	159	LEU
2	B	190	ASP
3	C	4	LEU
3	C	5	GLN
3	C	8	THR
3	C	10	VAL
3	C	15	SER
3	C	24	ASN
3	C	27	THR
3	C	30	SER
3	C	61	CYS
3	C	66	ASP
3	C	90	PHE
3	C	103	ASN
3	C	105	THR
3	C	117	THR
3	C	161	ILE
3	C	194	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	38	GLN
3	C	137	ASN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	C	303	3	14,14,15	0.89	1 (7%)	17,19,21	2.50	5 (29%)
4	NAG	C	305	4	14,14,15	0.63	0	17,19,21	1.48	3 (17%)
4	NAG	C	302	4	14,14,15	1.00	1 (7%)	17,19,21	1.31	3 (17%)
4	NAG	C	304	3,4	14,14,15	0.55	0	17,19,21	1.95	5 (29%)
4	NAG	C	301	3,4	14,14,15	0.59	0	17,19,21	1.42	3 (17%)

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	C	303	3	-	3/6/23/26	0/1/1/1
4	NAG	C	305	4	-	2/6/23/26	0/1/1/1
4	NAG	C	302	4	-	0/6/23/26	0/1/1/1
4	NAG	C	304	3,4	-	3/6/23/26	0/1/1/1
4	NAG	C	301	3,4	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	302	NAG	O6-C6	2.40	1.52	1.42
4	C	303	NAG	C1-C2	2.03	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	303	NAG	C2-N2-C7	6.08	131.56	122.90
4	C	303	NAG	C1-O5-C5	5.82	120.08	112.19
4	C	304	NAG	C2-N2-C7	4.76	129.68	122.90
4	C	305	NAG	C4-C3-C2	3.68	116.41	111.02
4	C	303	NAG	C4-C3-C2	-3.55	105.82	111.02
4	C	304	NAG	C1-C2-N2	3.53	116.52	110.49
4	C	305	NAG	C1-O5-C5	2.91	116.13	112.19
4	C	305	NAG	C2-N2-C7	2.84	126.95	122.90
4	C	301	NAG	C1-O5-C5	2.78	115.95	112.19
4	C	304	NAG	O5-C1-C2	-2.64	107.12	111.29
4	C	303	NAG	O3-C3-C2	2.57	114.78	109.47
4	C	304	NAG	C4-C3-C2	2.46	114.62	111.02
4	C	301	NAG	C2-N2-C7	2.45	126.39	122.90
4	C	302	NAG	O4-C4-C5	2.41	115.29	109.30
4	C	301	NAG	O4-C4-C5	2.36	115.16	109.30
4	C	303	NAG	O7-C7-N2	2.24	126.06	121.95
4	C	304	NAG	C8-C7-N2	-2.21	112.35	116.10
4	C	302	NAG	O5-C5-C6	2.16	110.59	107.20
4	C	302	NAG	O5-C5-C4	-2.05	105.84	110.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	303	NAG	C3-C2-N2-C7
4	C	304	NAG	O5-C5-C6-O6
4	C	305	NAG	O5-C5-C6-O6
4	C	304	NAG	C1-C2-N2-C7
4	C	304	NAG	C4-C5-C6-O6
4	C	303	NAG	O5-C5-C6-O6
4	C	303	NAG	C1-C2-N2-C7
4	C	305	NAG	C4-C5-C6-O6

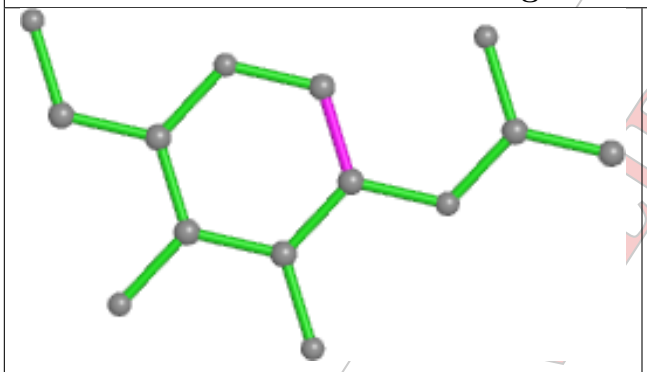
There are no ring outliers.

1 monomer is involved in 1 short contact:

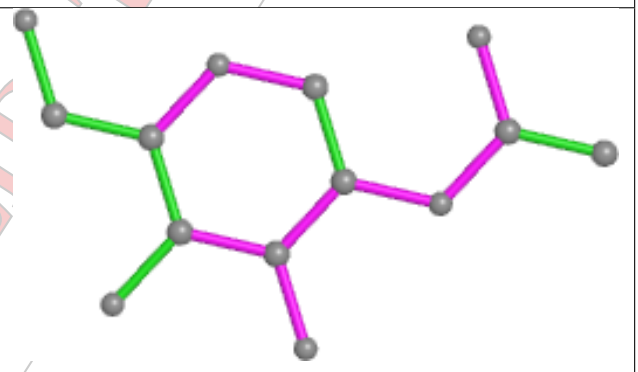
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	303	NAG	1	0

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.

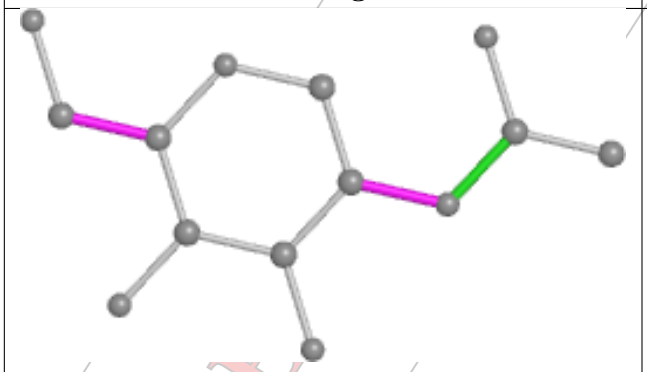
Ligand NAG C 303



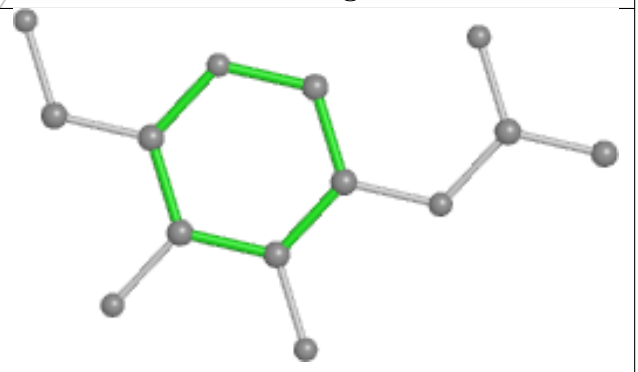
Bond lengths



Bond angles

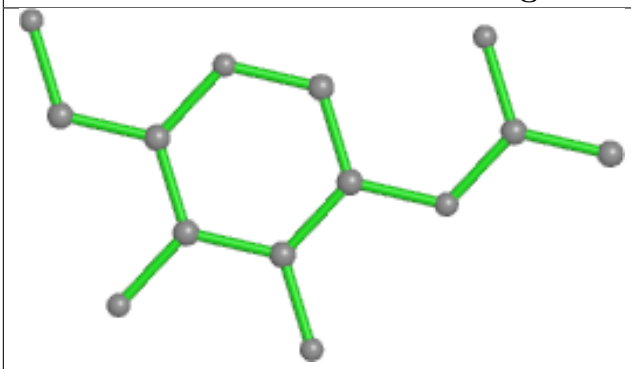


Torsions

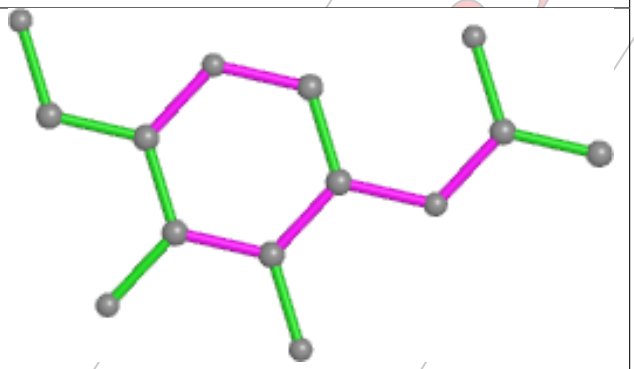


Rings

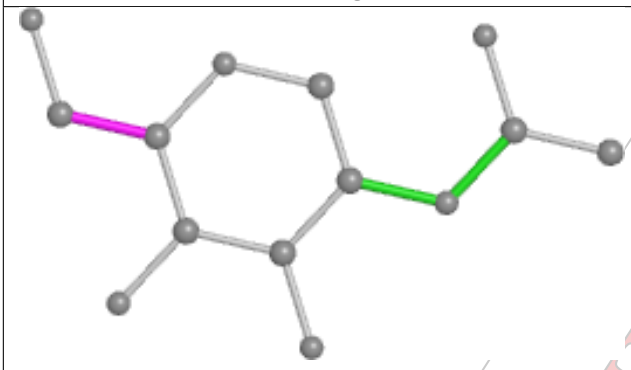
Ligand NAG C 305



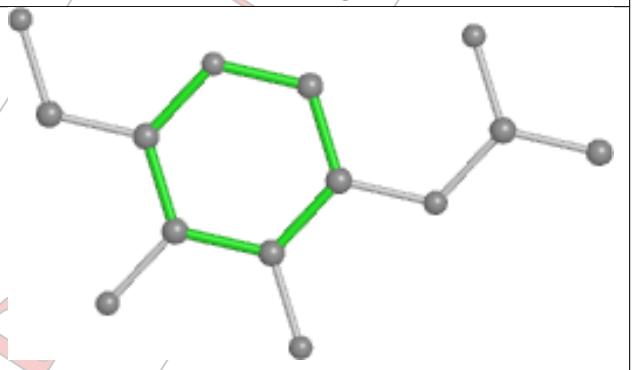
Bond lengths



Bond angles

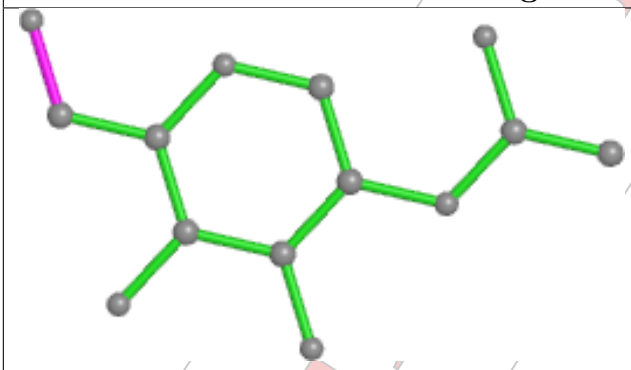


Torsions

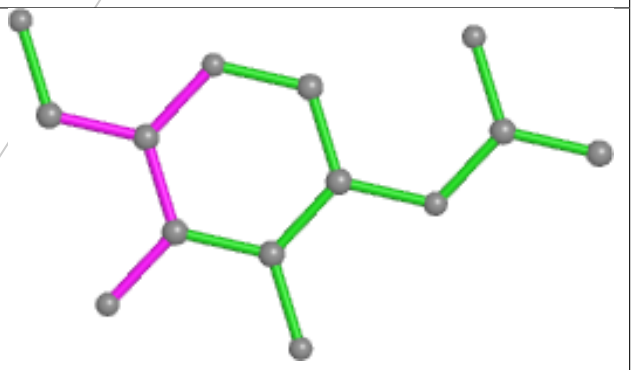


Rings

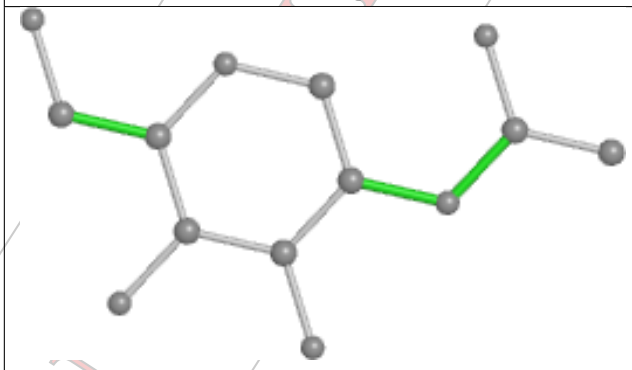
Ligand NAG C 302



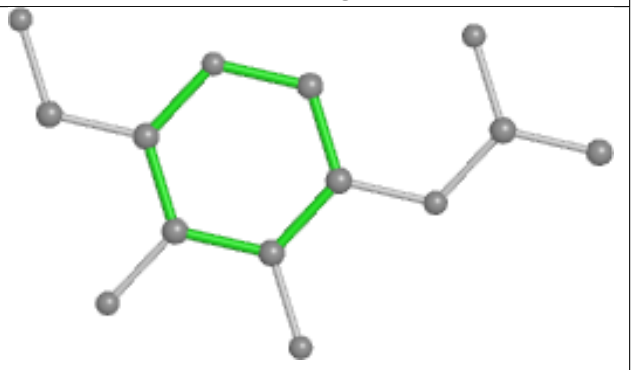
Bond lengths



Bond angles

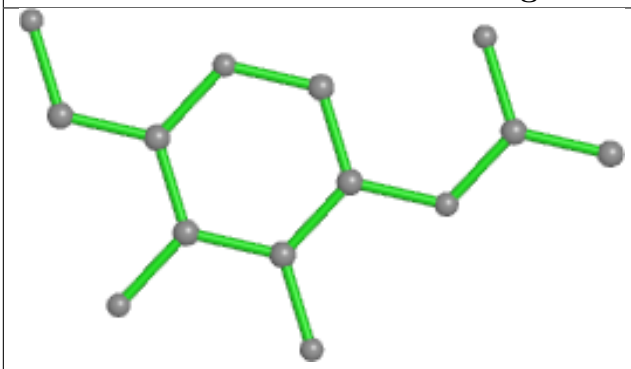


Torsions

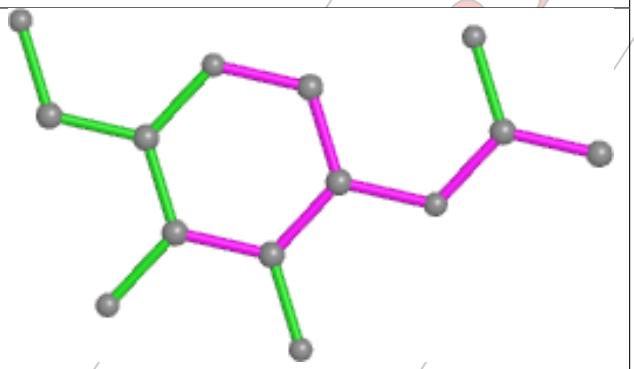


Rings

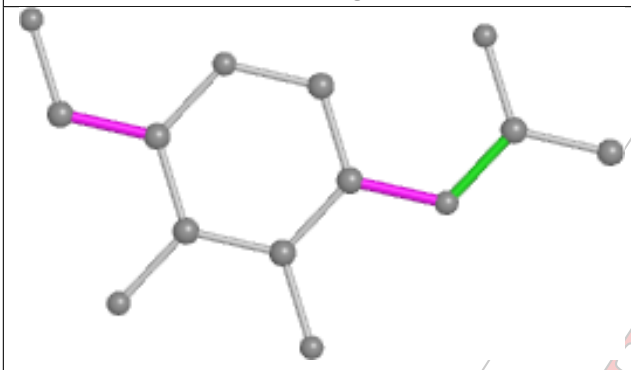
Ligand NAG C 304



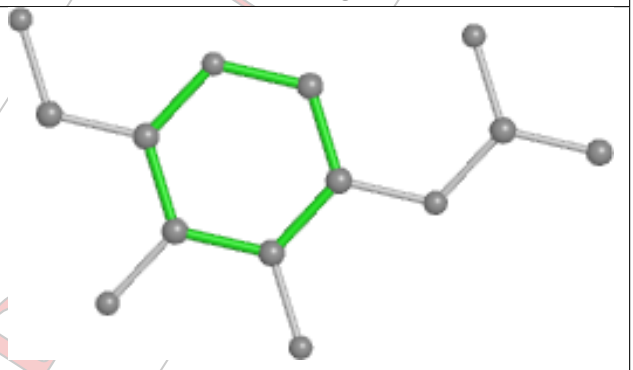
Bond lengths



Bond angles

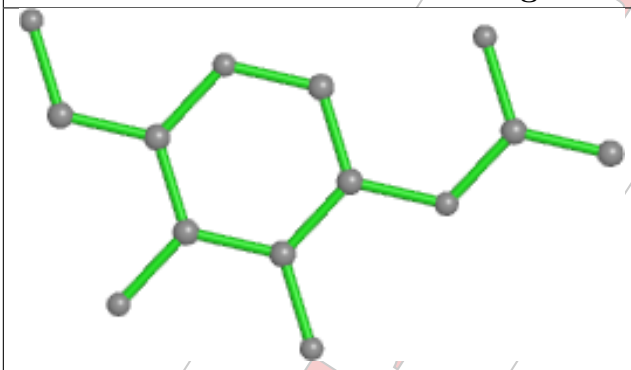


Torsions

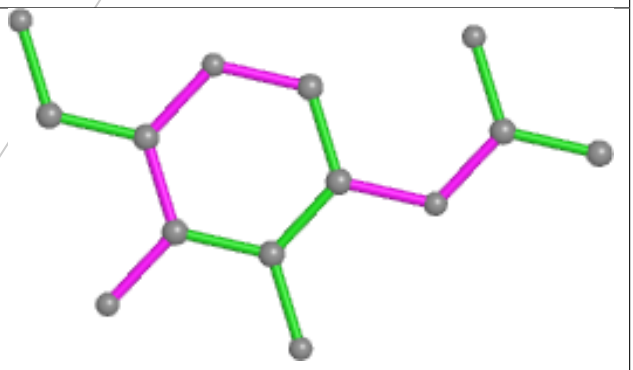


Rings

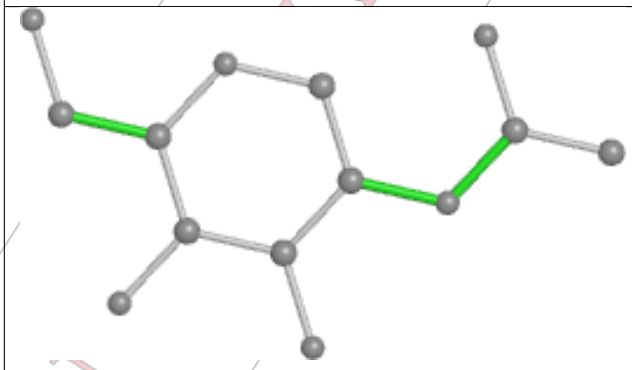
Ligand NAG C 301



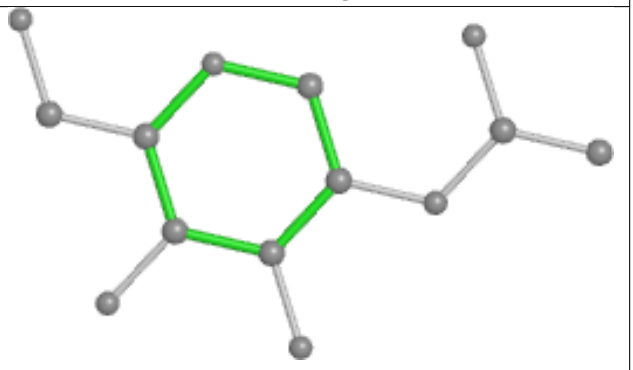
Bond lengths



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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	222/234 (94%)	0.39	2 (0%)	84	79	41, 67, 93, 114	0
2	B	216/217 (99%)	0.16	1 (0%)	90	88	43, 65, 97, 112	0
3	C	178/218 (81%)	0.51	8 (4%)	33	23	52, 75, 112, 131	0
All	All	616/669 (92%)	0.34	11 (1%)	68	60	41, 69, 102, 131	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	LEU	4.1
3	C	115	LEU	3.5
3	C	33	LEU	3.2
3	C	161	ILE	2.9
3	C	21	TRP	2.8
3	C	194	THR	2.8
3	C	36	LEU	2.5
1	A	150	LEU	2.5
2	B	138	VAL	2.2
3	C	138	ILE	2.2
3	C	116	LEU	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 carbohydrates in this entry.

6.4 Ligands (i)

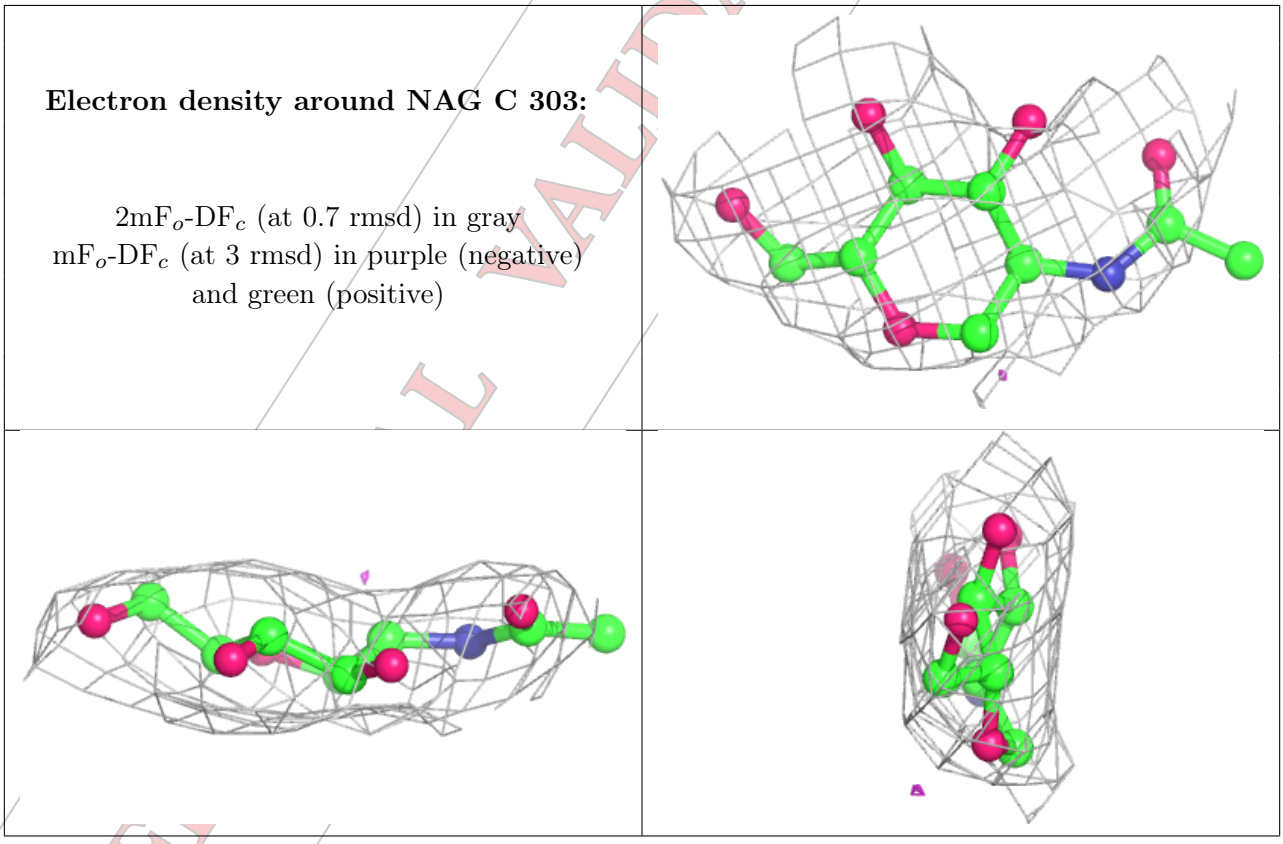
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	C	303	14/15	0.82	0.27	81,107,135,140	0
4	NAG	C	305	14/15	0.82	0.14	83,125,146,149	0
4	NAG	C	302	14/15	0.87	0.16	60,96,108,111	0
4	NAG	C	301	14/15	0.89	0.15	60,86,105,117	0
4	NAG	C	304	14/15	0.92	0.18	52,96,115,123	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.

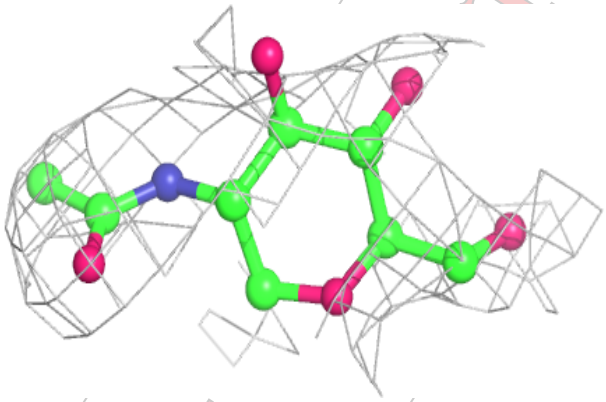
Electron density around NAG C 303:

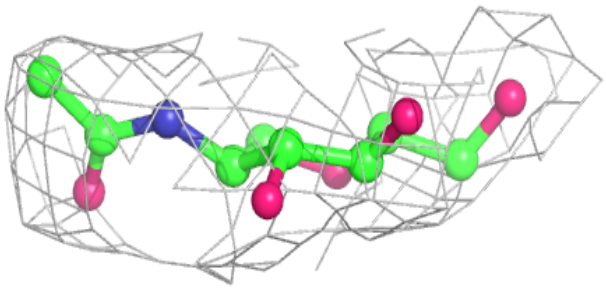
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

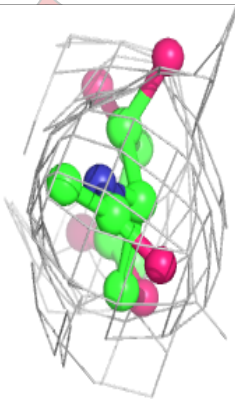


Electron density around NAG C 305:

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

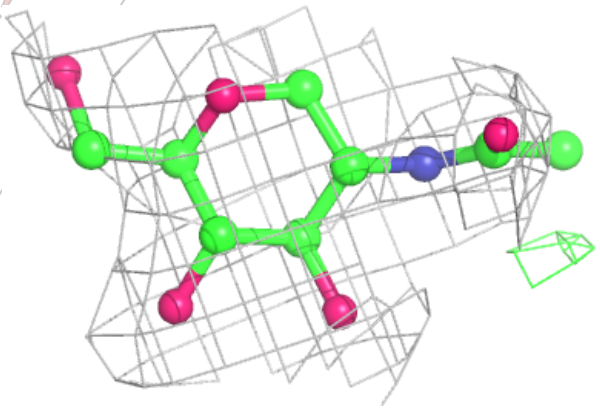


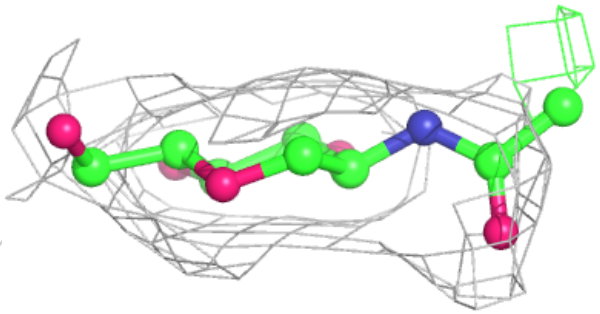


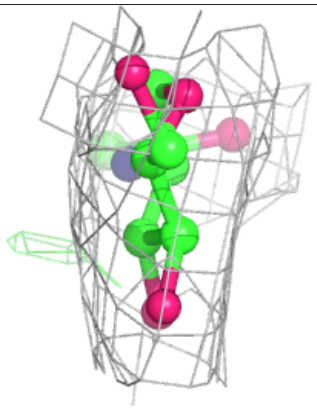


Electron density around NAG C 302:

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

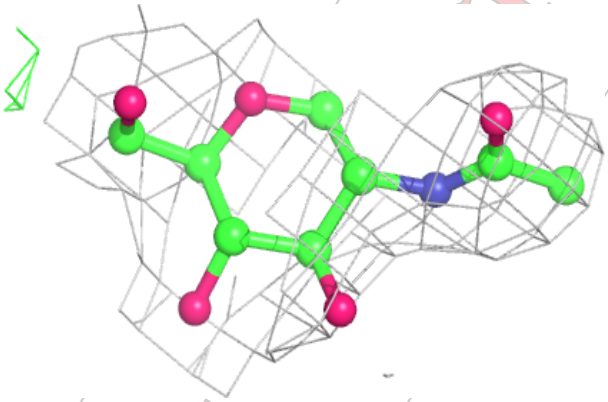


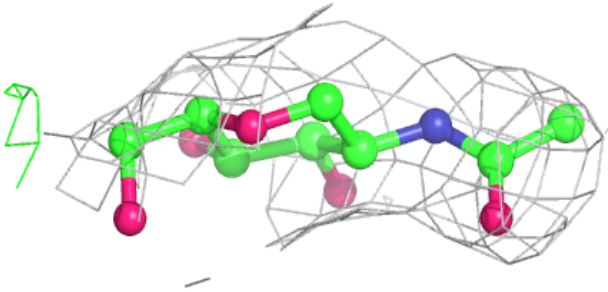


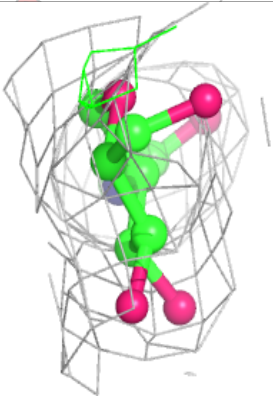


Electron density around NAG C 301:

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

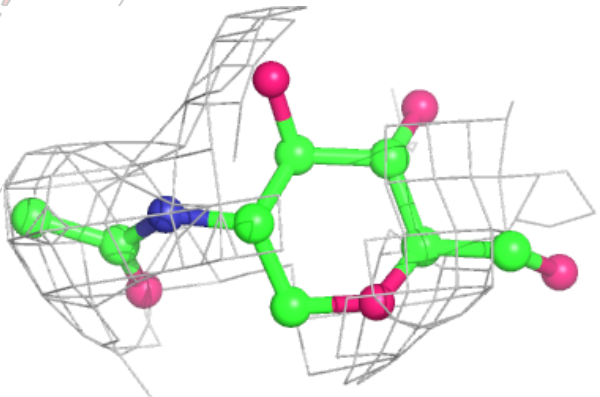


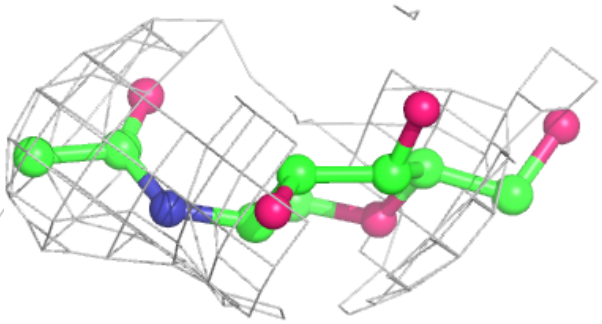


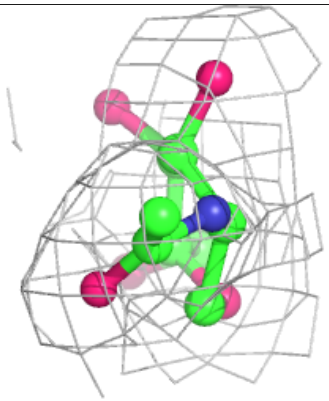


Electron density around NAG C 304:

$2mF_o$-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.