Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2020 – 12:00 PM BST

PDB ID	:	6VLD
Title	:	Crystal structure of human alpha 1,6-fucosyltransferase, FUT8 bound to GDP and A2SGP
Authors	:	Jarva, M.A.; Dramicanin, M.; Lingford, J.P.; Mao, R.; John, A.; Goddard-Borger, E.D.
Deposited on	:	2020-01-23
Resolution	:	2.28 Å(reported)

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	:	2.14.4.dev1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

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 2.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
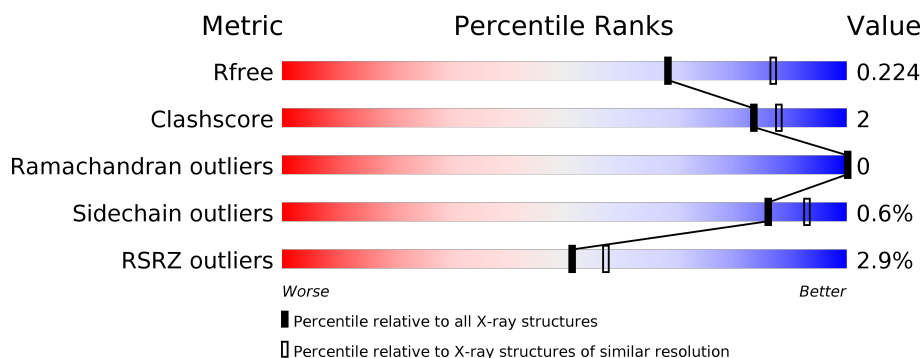
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	481	91% 6% ·
1	B	481	4% 90% 7% ·
1	G	481	6% 87% 10% ·
1	H	481	89% 5% 6%
2	C	7	86% 14%
2	D	7	71% 29%

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Mol	Chain	Length	Quality of chain
2	E	7	57% 43%
2	F	7	71% 29%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16219 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 Alpha-(1,6)-fucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3796	2416	669	697	14			
1	B	469	Total	C	N	O	S	0	0	0
			3814	2427	672	701	14			
1	G	465	Total	C	N	O	S	0	0	0
			3785	2410	667	694	14			
1	H	453	Total	C	N	O	S	0	0	0
			3688	2352	648	674	14			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	576	HIS	-	expression tag	UNP Q9BYC5
A	577	HIS	-	expression tag	UNP Q9BYC5
A	578	HIS	-	expression tag	UNP Q9BYC5
A	579	HIS	-	expression tag	UNP Q9BYC5
A	580	HIS	-	expression tag	UNP Q9BYC5
A	581	HIS	-	expression tag	UNP Q9BYC5
A	582	HIS	-	expression tag	UNP Q9BYC5
A	583	HIS	-	expression tag	UNP Q9BYC5
A	584	HIS	-	expression tag	UNP Q9BYC5
A	585	HIS	-	expression tag	UNP Q9BYC5
B	576	HIS	-	expression tag	UNP Q9BYC5
B	577	HIS	-	expression tag	UNP Q9BYC5
B	578	HIS	-	expression tag	UNP Q9BYC5
B	579	HIS	-	expression tag	UNP Q9BYC5
B	580	HIS	-	expression tag	UNP Q9BYC5
B	581	HIS	-	expression tag	UNP Q9BYC5
B	582	HIS	-	expression tag	UNP Q9BYC5
B	583	HIS	-	expression tag	UNP Q9BYC5
B	584	HIS	-	expression tag	UNP Q9BYC5
B	585	HIS	-	expression tag	UNP Q9BYC5
G	576	HIS	-	expression tag	UNP Q9BYC5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	577	HIS	-	expression tag	UNP Q9BYC5
G	578	HIS	-	expression tag	UNP Q9BYC5
G	579	HIS	-	expression tag	UNP Q9BYC5
G	580	HIS	-	expression tag	UNP Q9BYC5
G	581	HIS	-	expression tag	UNP Q9BYC5
G	582	HIS	-	expression tag	UNP Q9BYC5
G	583	HIS	-	expression tag	UNP Q9BYC5
G	584	HIS	-	expression tag	UNP Q9BYC5
G	585	HIS	-	expression tag	UNP Q9BYC5
H	576	HIS	-	expression tag	UNP Q9BYC5
H	577	HIS	-	expression tag	UNP Q9BYC5
H	578	HIS	-	expression tag	UNP Q9BYC5
H	579	HIS	-	expression tag	UNP Q9BYC5
H	580	HIS	-	expression tag	UNP Q9BYC5
H	581	HIS	-	expression tag	UNP Q9BYC5
H	582	HIS	-	expression tag	UNP Q9BYC5
H	583	HIS	-	expression tag	UNP Q9BYC5
H	584	HIS	-	expression tag	UNP Q9BYC5
H	585	HIS	-	expression tag	UNP Q9BYC5

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
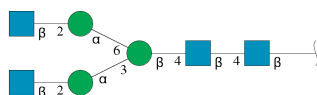
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			89	50	4	35			
2	D	7	Total	C	N	O	0	0	0
			89	50	4	35			
2	E	7	Total	C	N	O	0	0	0
			89	50	4	35			
2	F	7	Total	C	N	O	0	0	0
			89	50	4	35			

- Molecule 3 is ASPARAGINE (three-letter code: ASN) (formula: $C_4H_8N_2O_3$) (labeled as "Ligand of Interest" by author).

ASN
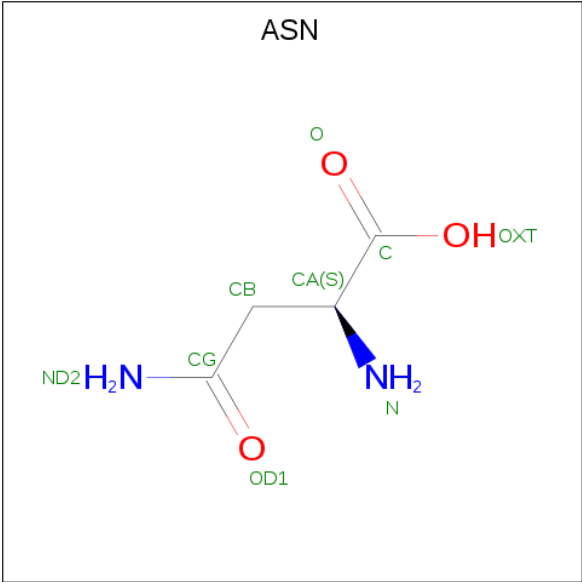
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 9	C 4	N 2	O 3	0	0
3	B	1	Total 9	C 4	N 2	O 3	0	0
3	G	1	Total 9	C 4	N 2	O 3	0	0
3	H	1	Total 9	C 4	N 2	O 3	0	0

- Molecule 4 is G U A N O S I N E - 5'- D I P H O S P H A T E (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by author).

GDP
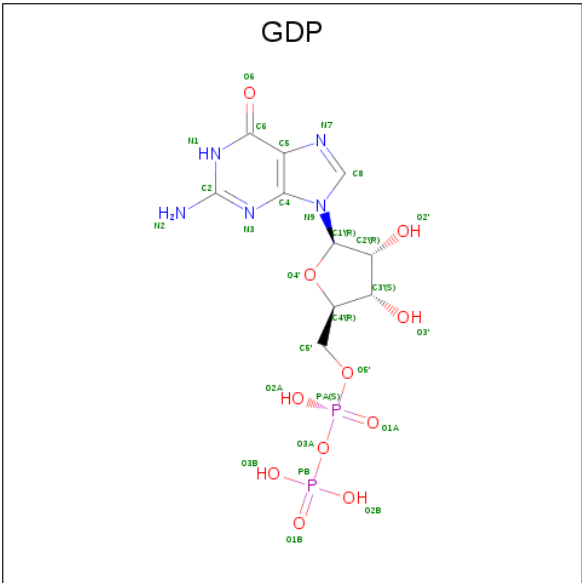
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
4	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
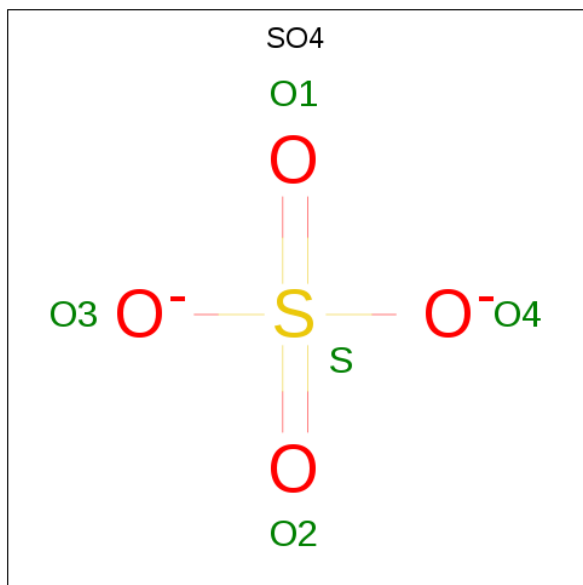
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total 5	O 4	S 1	0	0
5	H	1	Total 5	O 4	S 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	200	Total 200	O 200	0	0
6	B	87	Total 87	O 87	0	0
6	G	69	Total 69	O 69	0	0
6	H	272	Total 272	O 272	0	0

3 Residue-property plots ⓘ

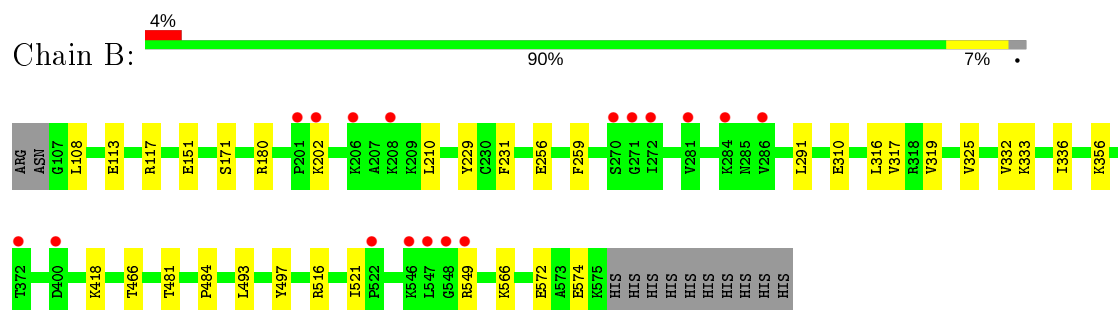These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.
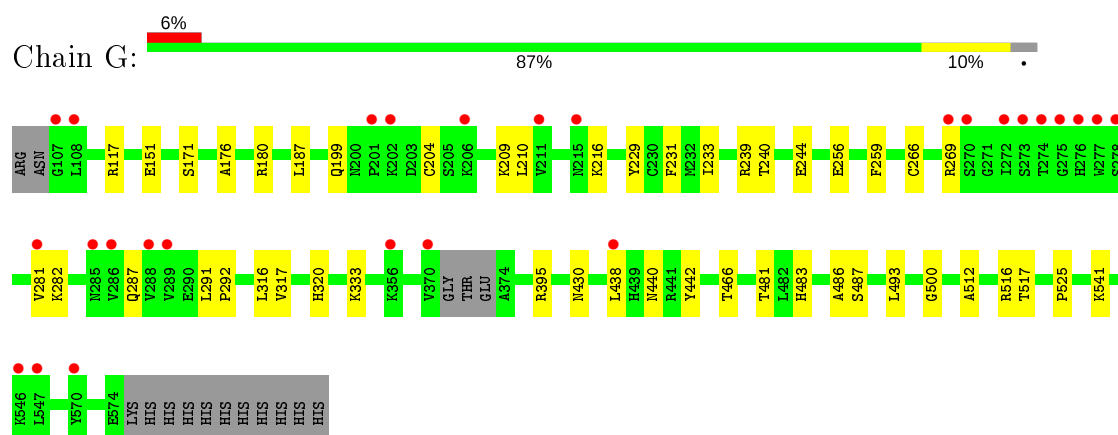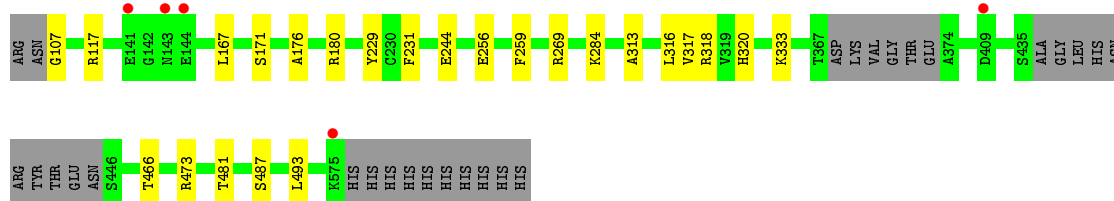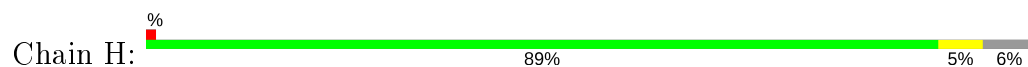
- Molecule 1: Alpha-(1,6)-fucosyltransferase
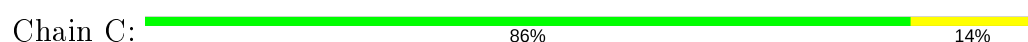

- Molecule 1: Alpha-(1,6)-fucosyltransferase

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Chain H:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
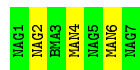
Chain E:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
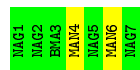
Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	208.31Å 68.45Å 249.98Å 90.00° 111.21° 90.00°	Depositor
Resolution (Å)	48.55 – 2.28 48.65 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.55-2.28) 99.9 (48.65-2.28)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.42 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.191 , 0.224 0.192 , 0.224	Depositor DCC
R_{free} test set	7492 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.7	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16219	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MAN, BMA, NAG, SO4

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	0.25	0/3896	0.40	0/5282
1	B	0.24	0/3914	0.40	0/5305
1	G	0.24	0/3884	0.39	0/5264
1	H	0.24	0/3784	0.40	0/5126
All	All	0.24	0/15478	0.40	0/20977

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3796	0	3708	17	0
1	B	3814	0	3727	23	0
1	G	3785	0	3697	30	0
1	H	3688	0	3610	16	0
2	C	89	0	76	0	0
2	D	89	0	76	0	0
2	E	89	0	76	1	0
2	F	89	0	76	0	0
3	A	9	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	4	0	0
3	G	9	0	4	0	0
3	H	9	0	4	0	0
4	A	28	0	12	0	0
4	B	28	0	12	0	0
5	A	20	0	0	0	0
5	B	5	0	0	0	0
5	G	10	0	0	1	0
5	H	25	0	0	0	0
6	A	200	0	0	1	0
6	B	87	0	0	2	0
6	G	69	0	0	2	0
6	H	272	0	0	2	0
All	All	16219	0	15086	74	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 2.

All (74) 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:G:209:LYS:NZ	1:G:266:CYS:SG	2.55	0.80
1:A:473:ARG:NH2	6:A:701:HOH:O	2.27	0.66
1:B:171:SER:O	1:B:180:ARG:NH2	2.29	0.66
1:B:210:LEU:HD11	1:B:291:LEU:HB2	1.78	0.64
1:G:395:ARG:NH2	6:G:702:HOH:O	2.31	0.62
1:G:438:LEU:O	1:G:440:ASN:ND2	2.32	0.61
1:H:466:THR:HG22	1:H:493:LEU:HB2	1.83	0.60
1:B:418:LYS:NZ	6:B:702:HOH:O	2.38	0.56
1:A:363:HIS:CE1	1:A:471:VAL:HB	2.40	0.56
1:G:171:SER:O	1:G:180:ARG:NH2	2.36	0.56
1:B:466:THR:HG22	1:B:493:LEU:HB2	1.89	0.55
1:G:244:GLU:HG3	1:G:269:ARG:HH21	1.71	0.55
1:H:473:ARG:NH2	6:H:701:HOH:O	2.21	0.54
1:A:365:ARG:NH1	1:A:366:ARG:O	2.41	0.54
1:B:180:ARG:HG2	1:B:484:PRO:HB2	1.91	0.53
1:A:416:GLU:HG2	1:A:420:LYS:HE2	1.91	0.53
1:A:108:LEU:HD11	1:H:176:ALA:HB1	1.90	0.52
1:A:120:GLU:HG2	1:H:167:LEU:HD13	1.92	0.52
1:A:317:VAL:O	1:H:117:ARG:NH2	2.35	0.52
1:B:108:LEU:HD11	1:G:176:ALA:HB1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLU:OE2	1:A:424:TYR:OH	2.22	0.51
1:H:284:LYS:NZ	6:H:708:HOH:O	2.45	0.50
1:A:466:THR:HG22	1:A:493:LEU:HB2	1.94	0.49
1:B:310:GLU:HG2	1:B:566:LYS:HA	1.94	0.49
1:G:204:CYS:SG	1:G:209:LYS:NZ	2.84	0.49
1:H:244:GLU:OE2	1:H:269:ARG:NH1	2.45	0.48
1:G:244:GLU:HG3	1:G:269:ARG:NH2	2.28	0.48
1:A:202:LYS:HB2	1:B:202:LYS:HE2	1.96	0.48
1:B:521:ILE:HG22	1:B:549:ARG:HG2	1.95	0.48
1:H:171:SER:O	1:H:180:ARG:NH2	2.33	0.48
1:B:180:ARG:HG3	1:B:319:VAL:HG23	1.95	0.47
1:B:317:VAL:O	1:G:117:ARG:NH2	2.39	0.47
1:A:171:SER:O	1:A:180:ARG:NH2	2.32	0.47
1:G:233:ILE:HD12	1:G:291:LEU:HD21	1.95	0.47
1:G:256:GLU:HA	1:G:259:PHE:O	2.14	0.47
1:B:516:ARG:NH1	1:G:151:GLU:HB3	2.29	0.47
1:G:291:LEU:HD12	1:G:292:PRO:HD2	1.95	0.47
1:G:512:ALA:HB2	1:G:525:PRO:HD3	1.97	0.46
1:B:325:VAL:HG22	1:B:497:TYR:CE2	2.50	0.46
1:B:256:GLU:HA	1:B:259:PHE:O	2.16	0.46
1:A:108:LEU:O	1:H:318:ARG:HD3	2.16	0.46
1:B:113:GLU:OE1	1:G:180:ARG:NH1	2.50	0.45
1:B:574:GLU:N	1:B:574:GLU:OE2	2.49	0.45
1:G:333:LYS:HB2	1:G:481:THR:HG21	1.99	0.45
1:G:466:THR:HG22	1:G:493:LEU:HB2	1.99	0.45
1:G:210:LEU:HD11	1:G:291:LEU:HB2	1.98	0.45
1:A:504:ALA:HB1	1:A:545:ARG:HH12	1.83	0.44
1:H:256:GLU:HA	1:H:259:PHE:O	2.16	0.44
1:B:572:GLU:H	1:B:572:GLU:CD	2.21	0.44
1:G:430:ASN:ND2	1:G:442:TYR:O	2.49	0.44
1:B:356:LYS:NZ	6:B:708:HOH:O	2.51	0.44
1:G:216:LYS:NZ	6:G:706:HOH:O	2.51	0.43
1:A:256:GLU:HA	1:A:259:PHE:O	2.19	0.43
1:G:320:HIS:CE1	1:G:487:SER:HB3	2.54	0.42
1:G:281:VAL:HG13	1:G:282:LYS:HD3	2.00	0.42
1:G:541:LYS:NZ	5:G:610:SO4:O3	2.39	0.42
1:B:332:VAL:O	1:B:336:ILE:HG12	2.19	0.42
1:G:483:HIS:HB2	1:G:486:ALA:HB2	2.01	0.42
1:B:333:LYS:HB2	1:B:481:THR:HG21	2.01	0.41
1:H:316:LEU:HD23	1:H:316:LEU:HA	1.91	0.41
1:H:244:GLU:OE2	1:H:269:ARG:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:313:ALA:O	1:H:317:VAL:HG23	2.21	0.41
1:G:500:GLY:HA3	2:E:2:NAG:C7	2.50	0.41
1:H:320:HIS:CE1	1:H:487:SER:HB3	2.56	0.41
1:G:187:LEU:HD13	1:G:316:LEU:HD23	2.03	0.41
1:A:137:LEU:HA	1:A:137:LEU:HD23	1.93	0.41
1:G:199:GLN:HA	1:G:240:THR:HG23	2.03	0.41
1:A:248:TRP:HB3	1:A:251:ALA:O	2.21	0.40
1:B:151:GLU:HB3	1:G:516:ARG:NH1	2.36	0.40
1:G:239:ARG:NH1	1:G:287:GLN:O	2.55	0.40
1:H:333:LYS:HB2	1:H:481:THR:HG21	2.03	0.40
1:B:316:LEU:HA	1:B:319:VAL:HG12	2.03	0.40
1:B:117:ARG:NH2	1:G:317:VAL:O	2.45	0.40
1:A:179:TRP:NE1	1:H:107:GLY:HA2	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	465/481 (97%)	447 (96%)	18 (4%)	0	100	100
1	B	467/481 (97%)	449 (96%)	18 (4%)	0	100	100
1	G	461/481 (96%)	447 (97%)	14 (3%)	0	100	100
1	H	447/481 (93%)	434 (97%)	13 (3%)	0	100	100
All	All	1840/1924 (96%)	1777 (97%)	63 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	409/423 (97%)	407 (100%)	2 (0%)	88	94
1	B	411/423 (97%)	409 (100%)	2 (0%)	88	94
1	G	408/423 (96%)	405 (99%)	3 (1%)	84	91
1	H	398/423 (94%)	396 (100%)	2 (0%)	88	94
All	All	1626/1692 (96%)	1617 (99%)	9 (1%)	86	93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	TYR
1	A	231	PHE
1	B	229	TYR
1	B	231	PHE
1	G	229	TYR
1	G	231	PHE
1	G	517	THR
1	H	229	TYR
1	H	231	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	363	HIS
1	B	226	HIS
1	B	363	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

28 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	NAG	C	1	3,2	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	C	2	2	14,14,15	0.24	0	17,19,21	0.36	0
2	BMA	C	3	2	11,11,12	0.74	0	15,15,17	0.67	0
2	MAN	C	4	2	11,11,12	0.71	0	15,15,17	1.08	2 (13%)
2	NAG	C	5	2	14,14,15	0.18	0	17,19,21	0.45	0
2	MAN	C	6	2	11,11,12	0.86	0	15,15,17	0.98	0
2	NAG	C	7	2	14,14,15	0.31	0	17,19,21	0.39	0
2	NAG	D	1	3,2	14,14,15	0.20	0	17,19,21	0.44	0
2	NAG	D	2	2	14,14,15	0.30	0	17,19,21	0.36	0
2	BMA	D	3	2	11,11,12	0.72	0	15,15,17	0.71	0
2	MAN	D	4	2	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
2	NAG	D	5	2	14,14,15	0.23	0	17,19,21	0.39	0
2	MAN	D	6	2	11,11,12	0.74	0	15,15,17	1.05	2 (13%)
2	NAG	D	7	2	14,14,15	0.25	0	17,19,21	0.38	0
2	NAG	E	1	3,2	14,14,15	0.24	0	17,19,21	0.39	0
2	NAG	E	2	2	14,14,15	0.26	0	17,19,21	0.36	0
2	BMA	E	3	2	11,11,12	0.69	0	15,15,17	0.70	0
2	MAN	E	4	2	11,11,12	0.76	0	15,15,17	1.03	2 (13%)
2	NAG	E	5	2	14,14,15	0.24	0	17,19,21	0.40	0
2	MAN	E	6	2	11,11,12	0.77	0	15,15,17	1.05	2 (13%)
2	NAG	E	7	2	14,14,15	0.28	0	17,19,21	0.38	0
2	NAG	F	1	3,2	14,14,15	0.38	0	17,19,21	0.43	0
2	NAG	F	2	2	14,14,15	0.39	0	17,19,21	0.37	0
2	BMA	F	3	2	11,11,12	0.73	0	15,15,17	0.70	0
2	MAN	F	4	2	11,11,12	0.71	0	15,15,17	1.13	2 (13%)
2	NAG	F	5	2	14,14,15	0.31	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	MAN	F	6	2	11,11,12	0.90	0	15,15,17	1.08	1 (6%)
2	NAG	F	7	2	14,14,15	0.33	0	17,19,21	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	3,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	NAG	C	5	2	-	2/6/23/26	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	NAG	C	7	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	3,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	NAG	D	5	2	-	2/6/23/26	0/1/1/1
2	MAN	D	6	2	-	0/2/19/22	0/1/1/1
2	NAG	D	7	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	3,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	NAG	E	5	2	-	2/6/23/26	0/1/1/1
2	MAN	E	6	2	-	0/2/19/22	0/1/1/1
2	NAG	E	7	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	3,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	MAN	F	4	2	-	0/2/19/22	0/1/1/1
2	NAG	F	5	2	-	2/6/23/26	0/1/1/1
2	MAN	F	6	2	-	0/2/19/22	0/1/1/1
2	NAG	F	7	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4	MAN	O2-C2-C3	-2.61	104.91	110.14
2	F	4	MAN	C1-O5-C5	2.54	115.63	112.19
2	D	4	MAN	C1-O5-C5	2.49	115.57	112.19
2	C	4	MAN	C1-O5-C5	2.46	115.52	112.19
2	F	4	MAN	O2-C2-C3	-2.37	105.40	110.14
2	D	6	MAN	C1-O5-C5	2.37	115.40	112.19
2	E	4	MAN	C1-O5-C5	2.34	115.36	112.19
2	F	6	MAN	C1-O5-C5	2.26	115.25	112.19
2	D	4	MAN	O2-C2-C3	-2.22	105.69	110.14
2	E	6	MAN	C1-O5-C5	2.11	115.06	112.19
2	E	4	MAN	O2-C2-C3	-2.06	106.00	110.14
2	D	6	MAN	O2-C2-C3	-2.06	106.01	110.14
2	E	6	MAN	O2-C2-C3	-2.03	106.07	110.14

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	5	NAG	C8-C7-N2-C2
2	C	5	NAG	O7-C7-N2-C2
2	D	5	NAG	C8-C7-N2-C2
2	D	5	NAG	O7-C7-N2-C2
2	F	5	NAG	C8-C7-N2-C2
2	F	5	NAG	O7-C7-N2-C2
2	E	5	NAG	C8-C7-N2-C2
2	E	5	NAG	O7-C7-N2-C2
2	E	7	NAG	C4-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	E	7	NAG	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	D	7	NAG	C4-C5-C6-O6
2	D	7	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings
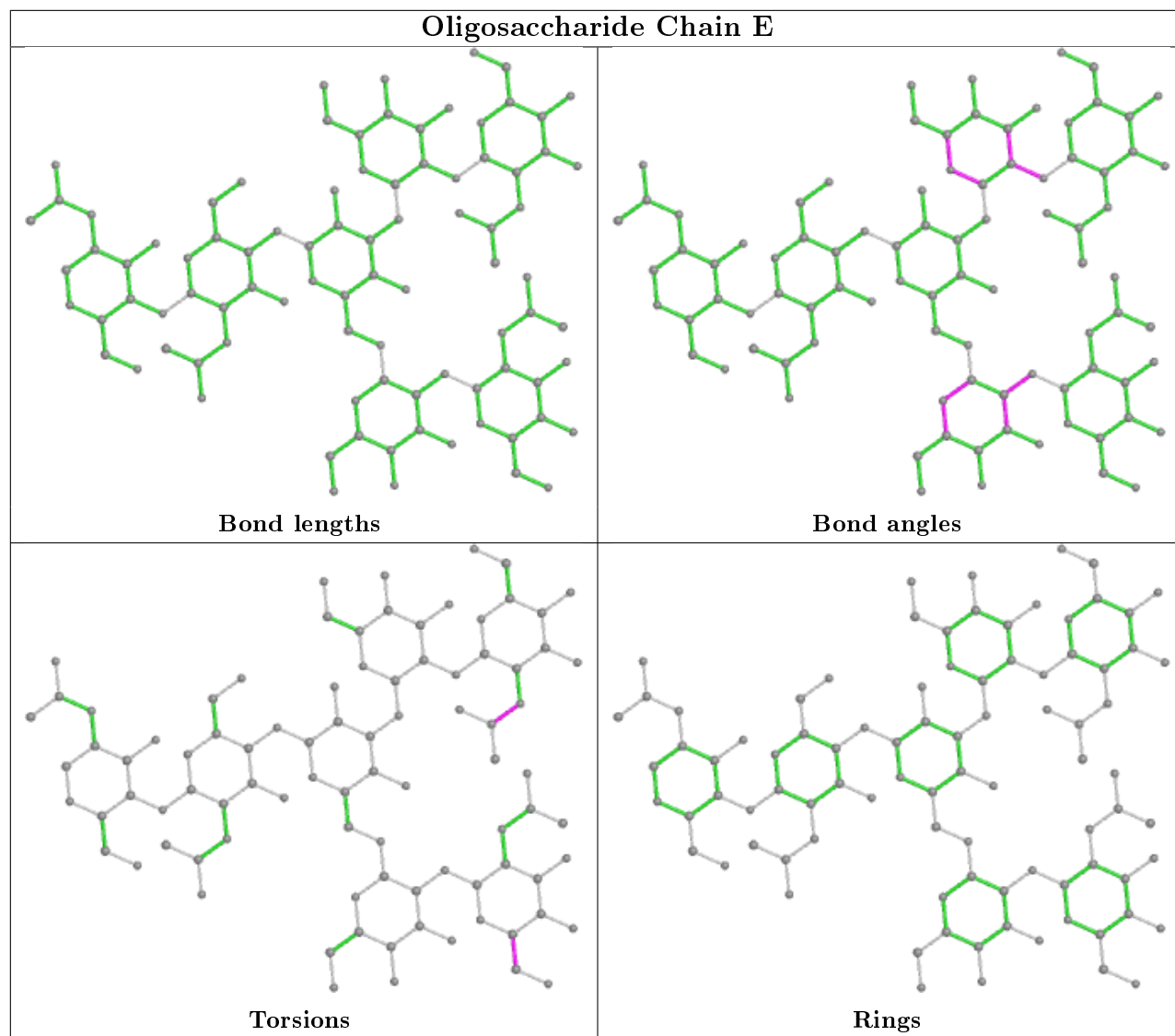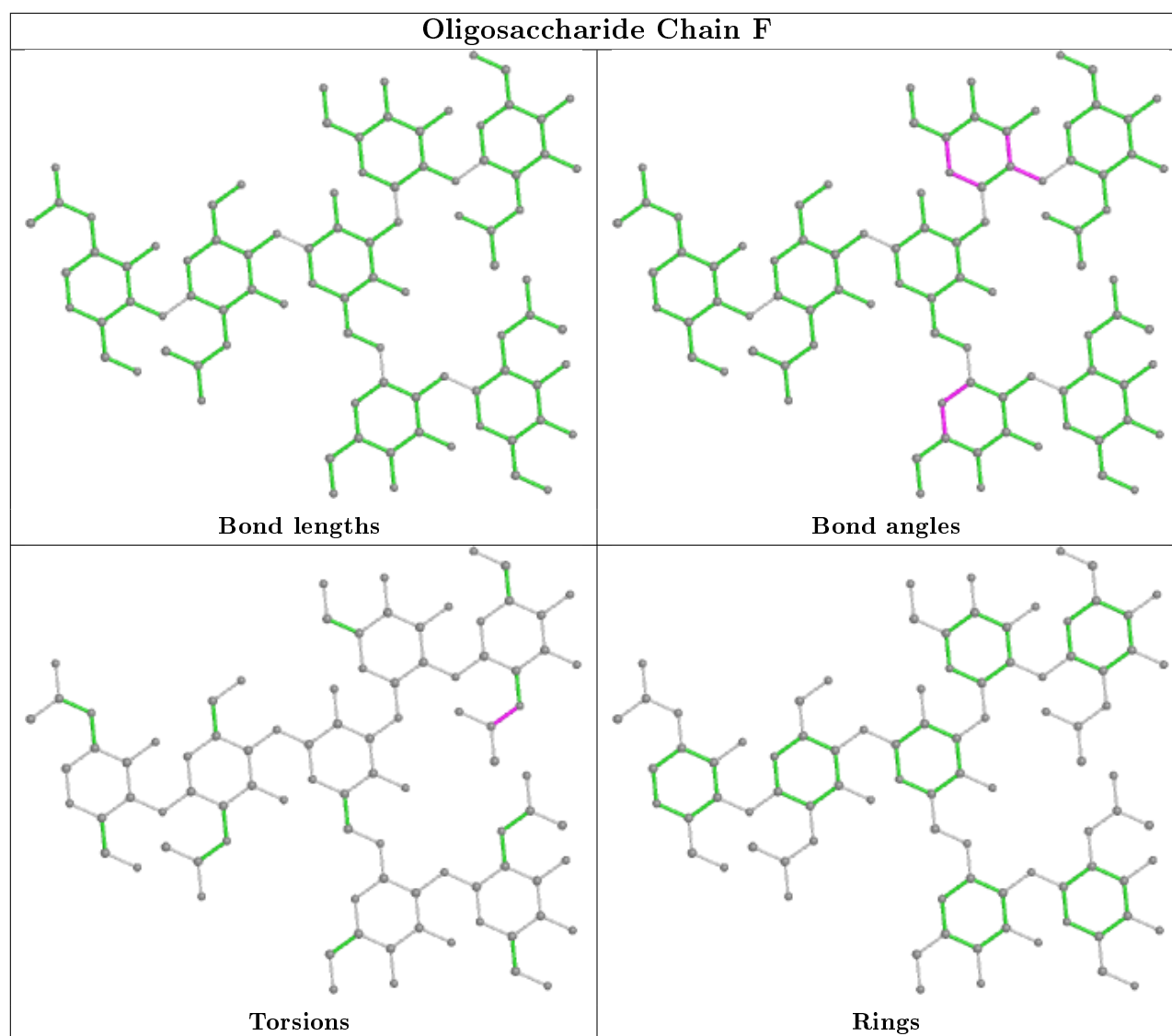
5.6 Ligand geometry ⓘ

18 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	GDP	A	609	-	24,30,30	1.19	2 (8%)	31,47,47	1.93	8 (25%)
4	GDP	B	609	-	24,30,30	1.19	2 (8%)	31,47,47	1.92	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	SO4	G	609	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	A	610	-	4,4,4	0.14	0	6,6,6	0.05	0
3	ASN	B	601	2	5,8,8	0.18	0	5,10,10	0.21	0
5	SO4	G	610	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	H	611	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	H	612	-	4,4,4	0.14	0	6,6,6	0.06	0
3	ASN	H	601	2	5,8,8	0.18	0	5,10,10	0.16	0
5	SO4	H	613	-	4,4,4	0.15	0	6,6,6	0.13	0
5	SO4	A	611	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	613	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	H	609	-	4,4,4	0.14	0	6,6,6	0.05	0
3	ASN	G	601	2	5,8,8	0.21	0	5,10,10	0.22	0
3	ASN	A	601	2	5,8,8	0.19	0	5,10,10	0.31	0
5	SO4	B	610	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	H	610	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	A	612	-	4,4,4	0.14	0	6,6,6	0.04	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GDP	A	609	-	-	4/12/32/32	0/3/3/3
4	GDP	B	609	-	-	4/12/32/32	0/3/3/3
3	ASN	B	601	2	-	2/4/8/8	-
3	ASN	H	601	2	-	0/4/8/8	-
3	ASN	G	601	2	-	2/4/8/8	-
3	ASN	A	601	2	-	0/4/8/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	609	GDP	C6-C5	4.23	1.48	1.41
4	B	609	GDP	C6-C5	4.18	1.48	1.41
4	A	609	GDP	C5-C4	2.44	1.47	1.40
4	B	609	GDP	C5-C4	2.38	1.47	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	609	GDP	C2-N3-C4	5.00	121.07	115.36
4	A	609	GDP	C2-N3-C4	5.00	121.07	115.36
4	A	609	GDP	C6-N1-C2	4.01	122.30	115.93
4	B	609	GDP	C6-N1-C2	4.01	122.29	115.93
4	A	609	GDP	C6-C5-C4	-3.96	117.02	120.80
4	B	609	GDP	C6-C5-C4	-3.93	117.04	120.80
4	B	609	GDP	C5-C6-N1	-3.91	118.08	123.43
4	A	609	GDP	C5-C6-N1	-3.88	118.12	123.43
4	B	609	GDP	N3-C2-N1	-3.36	122.74	127.22
4	A	609	GDP	N3-C2-N1	-3.31	122.81	127.22
4	A	609	GDP	C4-C5-N7	-2.78	106.50	109.40
4	B	609	GDP	C4-C5-N7	-2.75	106.53	109.40
4	B	609	GDP	PA-O3A-PB	-2.75	123.40	132.83
4	A	609	GDP	PA-O3A-PB	-2.70	123.55	132.83
4	A	609	GDP	O3B-PB-O3A	2.25	112.17	104.64
4	B	609	GDP	O3B-PB-O3A	2.14	111.81	104.64

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	609	GDP	C5'-O5'-PA-O3A
4	A	609	GDP	C5'-O5'-PA-O1A
4	B	609	GDP	C5'-O5'-PA-O3A
4	B	609	GDP	C5'-O5'-PA-O1A
4	B	609	GDP	C5'-O5'-PA-O2A
3	G	601	ASN	N-CA-CB-CG
4	A	609	GDP	C5'-O5'-PA-O2A
3	B	601	ASN	C-CA-CB-CG
3	G	601	ASN	C-CA-CB-CG
3	B	601	ASN	N-CA-CB-CG
4	A	609	GDP	O4'-C4'-C5'-O5'
4	B	609	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

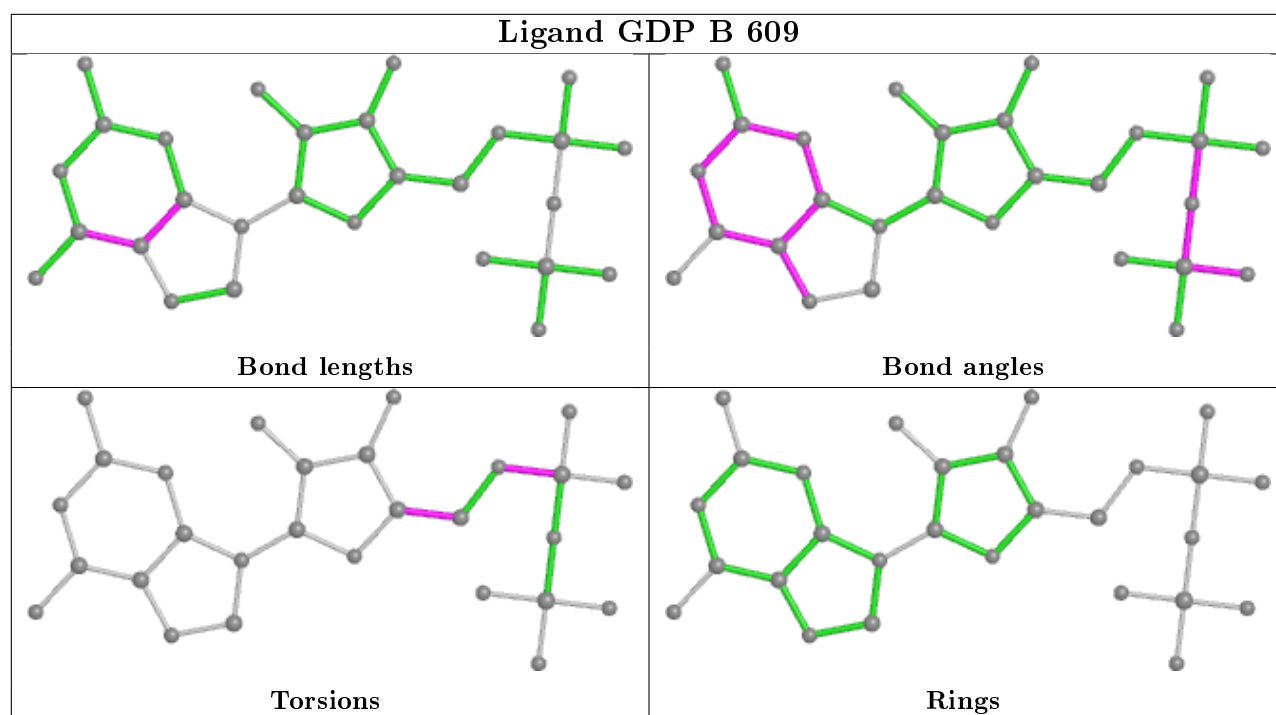1 monomer is involved in 1 short contact:

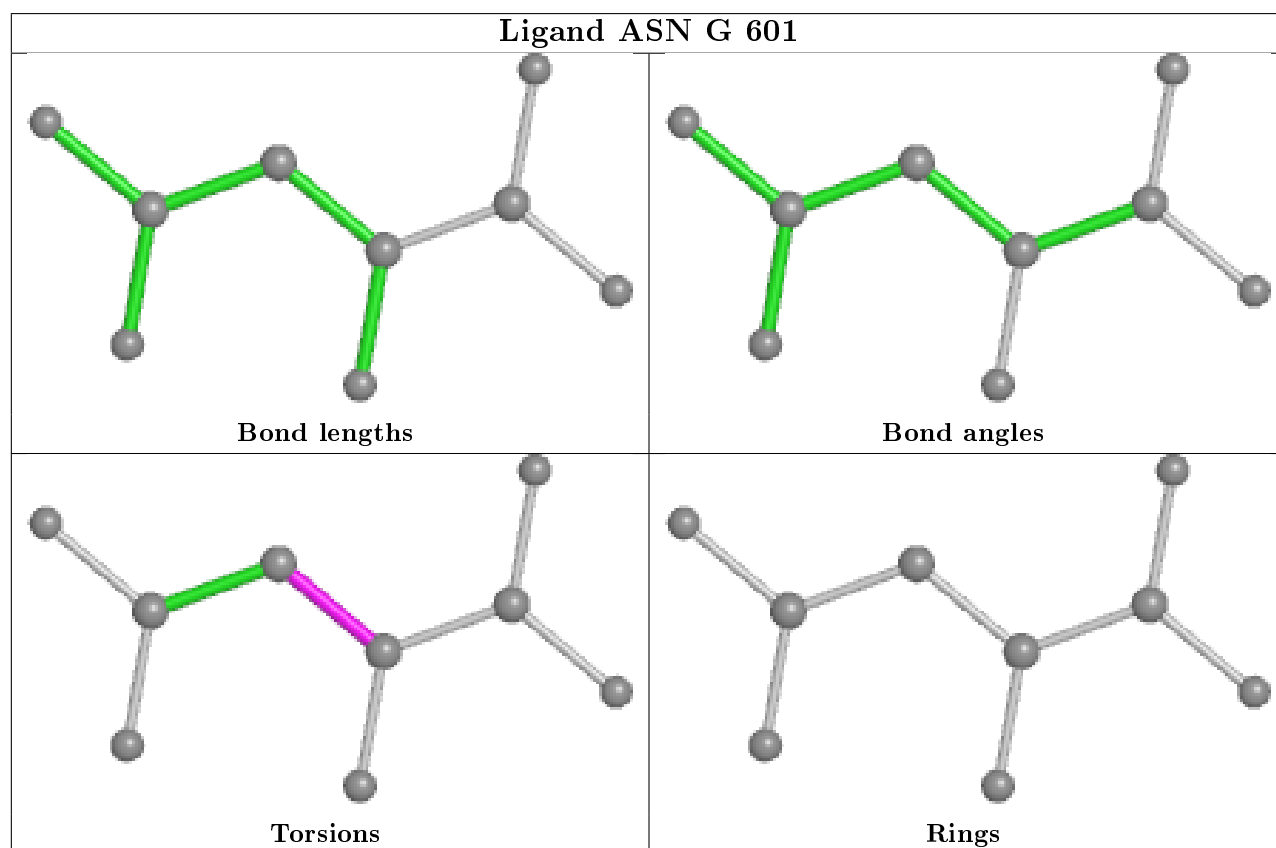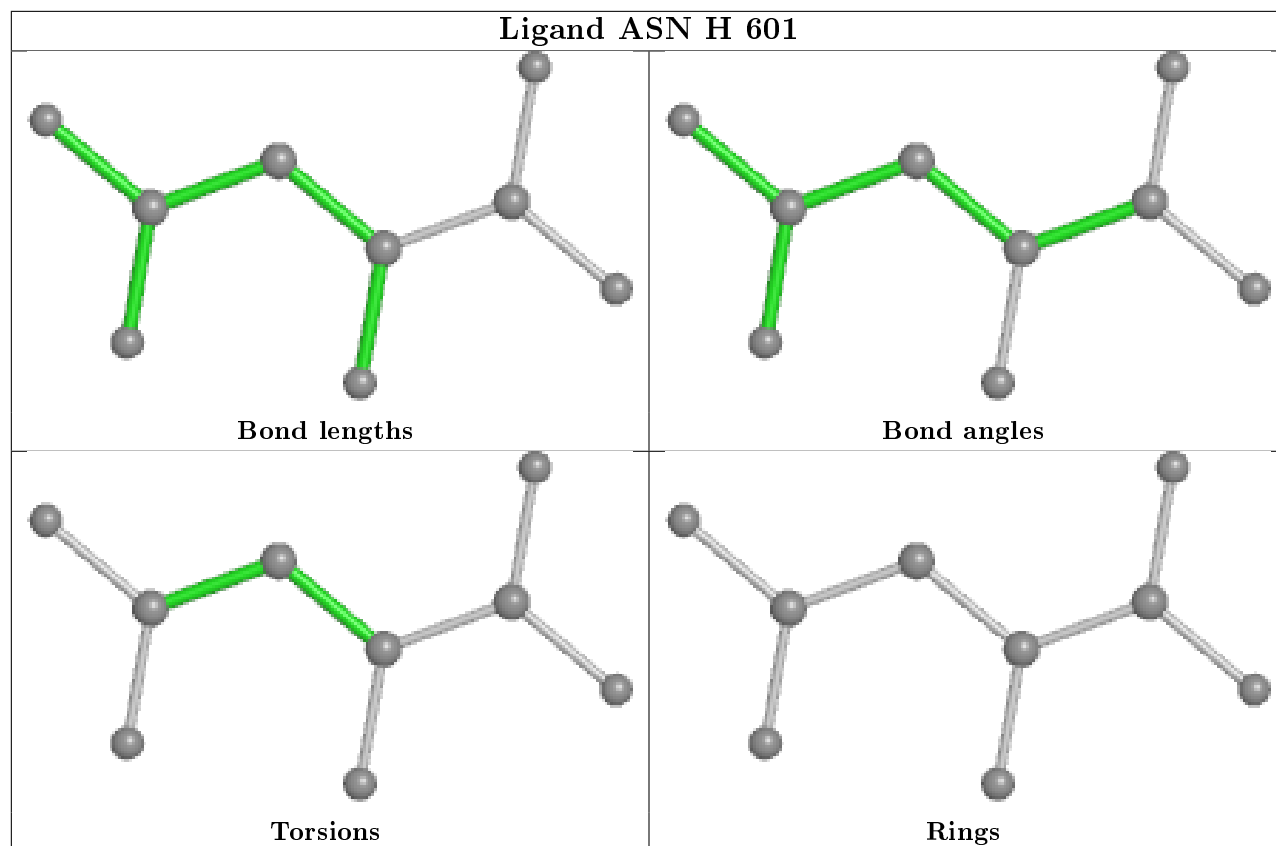| Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	610	SO4	1	0

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
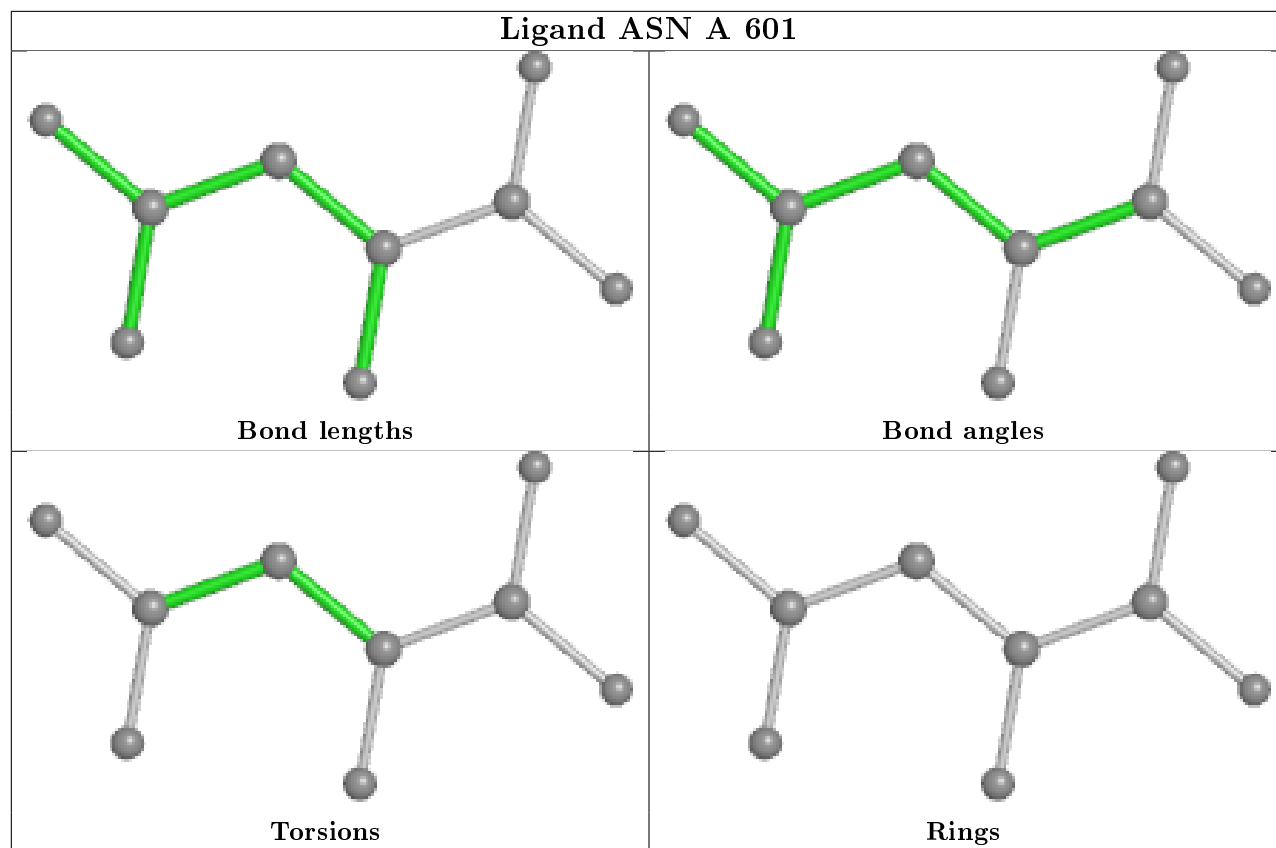
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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 GDP A 609

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP B 609

Bond lengths

Bond angles

Torsions

Rings

Ligand ASN B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ASN H 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ASN G 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ASN A 601
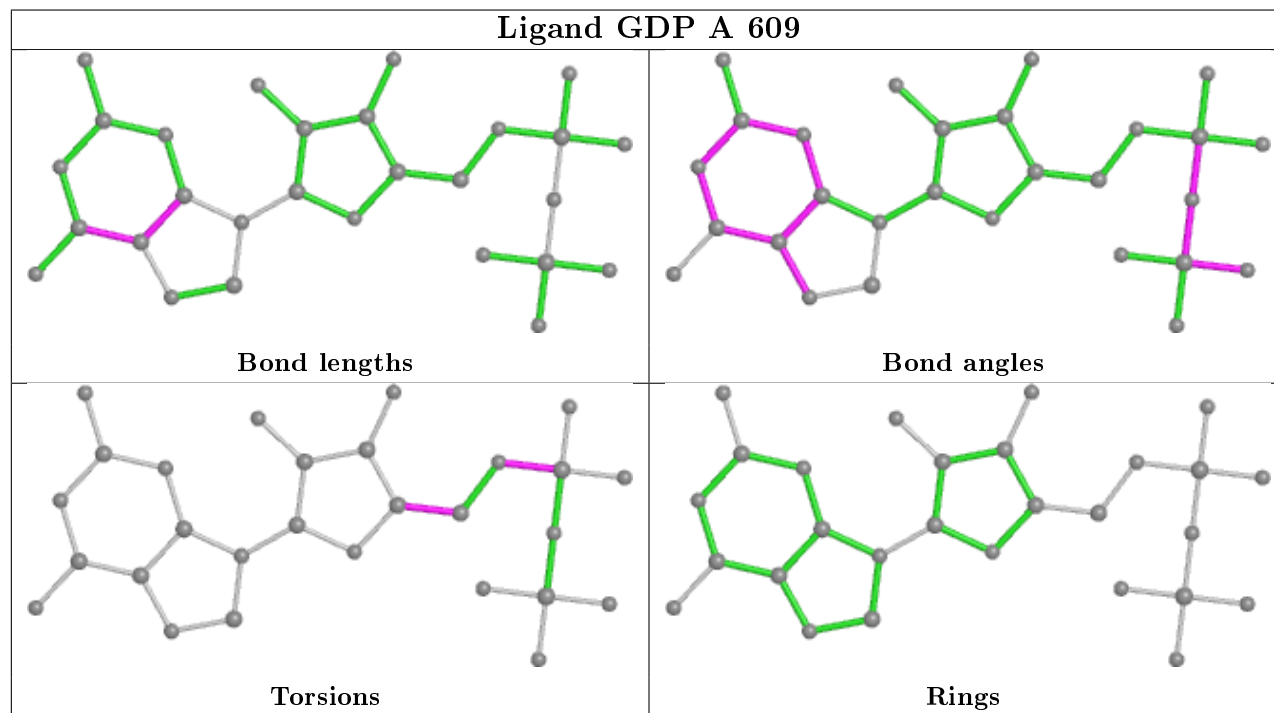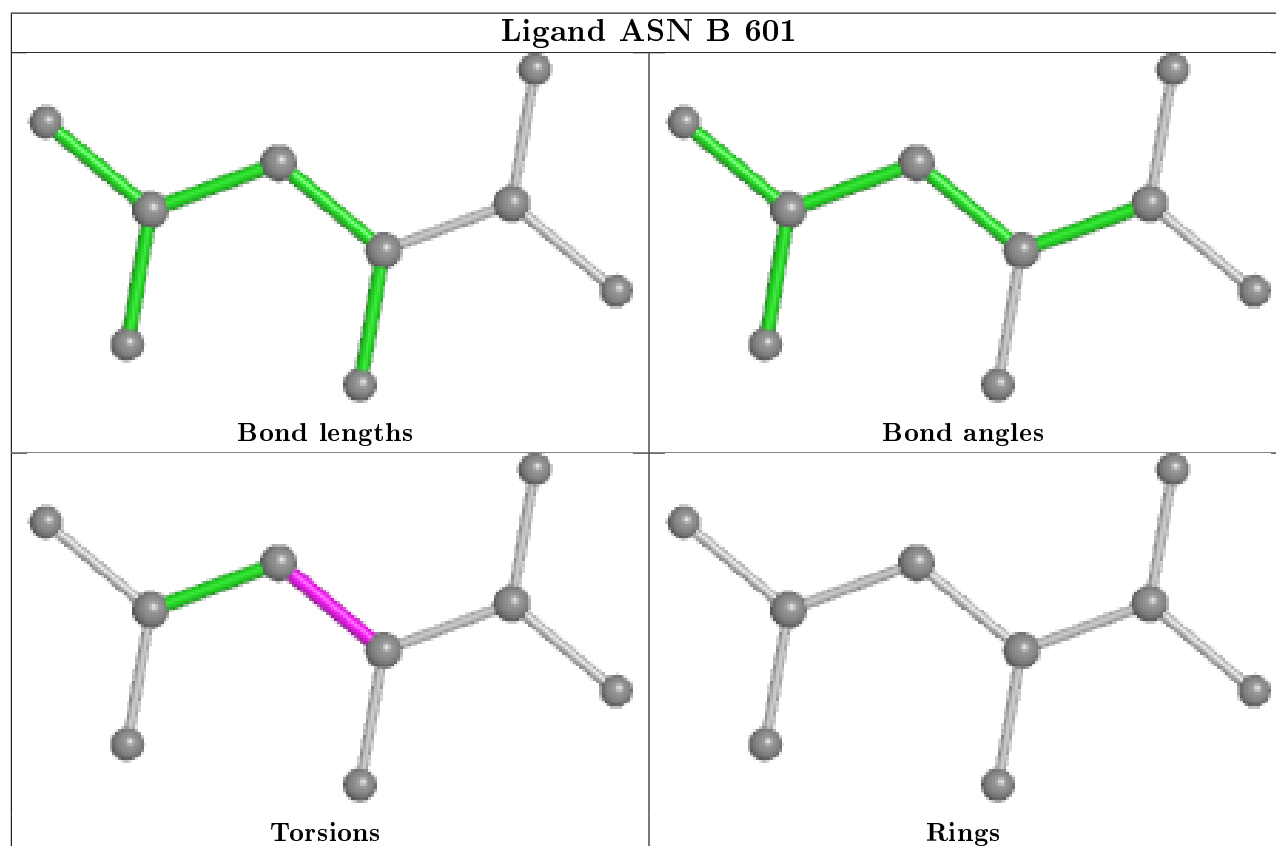
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	467/481 (97%)	-0.01	4 (0%)	84	87	38, 56, 83, 114	0
1	B	469/481 (97%)	0.16	17 (3%)	42	48	48, 68, 102, 127	0
1	G	465/481 (96%)	0.18	27 (5%)	23	28	52, 70, 109, 134	0
1	H	453/481 (94%)	-0.10	5 (1%)	80	84	33, 46, 82, 113	0
All	All	1854/1924 (96%)	0.06	53 (2%)	51	57	33, 62, 99, 134	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	206	LYS	5.7
1	G	289	VAL	5.6
1	G	107	GLY	5.6
1	G	272	ILE	4.5
1	B	372	THR	4.0
1	B	270	SER	4.0
1	G	288	VAL	4.0
1	G	370	VAL	3.9
1	G	281	VAL	3.8
1	B	202	LYS	3.6
1	G	269	ARG	3.5
1	G	273	SER	3.4
1	B	284	LYS	3.2
1	H	575	LYS	3.2
1	G	286	VAL	3.1
1	B	286	VAL	3.0
1	G	211	VAL	3.0
1	A	372	THR	3.0
1	G	438	LEU	3.0
1	B	271	GLY	3.0
1	B	281	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	215	ASN	2.9
1	G	201	PRO	2.8
1	B	548	GLY	2.8
1	G	274	THR	2.8
1	B	272	ILE	2.8
1	A	371	GLY	2.7
1	G	206	LYS	2.7
1	G	270	SER	2.7
1	G	108	LEU	2.7
1	A	400	ASP	2.6
1	G	275	GLY	2.6
1	H	141	GLU	2.6
1	G	278	SER	2.5
1	B	201	PRO	2.5
1	G	277	TRP	2.5
1	G	570	TYR	2.5
1	G	202	LYS	2.3
1	B	208	LYS	2.3
1	B	522	PRO	2.3
1	H	143	ASN	2.3
1	A	519	ASP	2.3
1	G	546	LYS	2.2
1	G	285	ASN	2.2
1	G	276	HIS	2.2
1	B	546	LYS	2.1
1	G	547	LEU	2.1
1	B	547	LEU	2.1
1	B	400	ASP	2.1
1	H	409	ASP	2.1
1	H	144	GLU	2.0
1	G	356	LYS	2.0
1	B	549	ARG	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
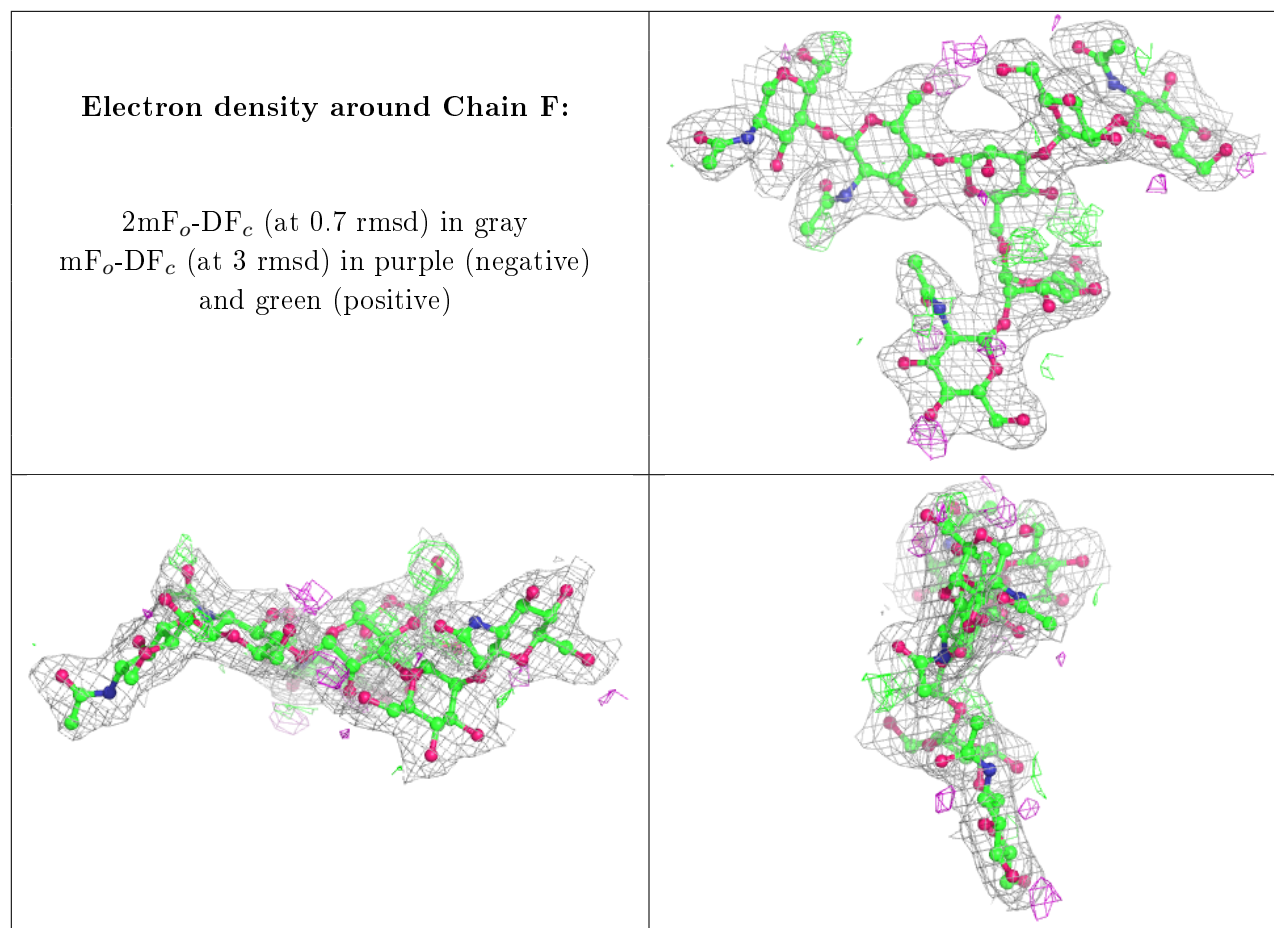
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	E	7	14/15	0.90	0.16	82,86,90,91	0
2	MAN	C	4	11/12	0.92	0.15	52,61,69,74	0
2	NAG	D	1	14/15	0.94	0.16	63,70,78,80	0
2	MAN	C	6	11/12	0.95	0.09	51,58,65,65	0
2	NAG	F	1	14/15	0.95	0.12	46,53,62,74	0
2	NAG	C	5	14/15	0.95	0.09	46,59,67,73	0
2	NAG	C	7	14/15	0.95	0.14	48,61,67,72	0
2	NAG	D	7	14/15	0.95	0.19	74,86,89,90	0
2	NAG	C	1	14/15	0.95	0.11	43,57,67,69	0
2	NAG	E	1	14/15	0.95	0.14	61,75,81,86	0
2	NAG	D	5	14/15	0.95	0.12	56,60,73,75	0
2	NAG	E	5	14/15	0.95	0.12	61,66,73,74	0
2	MAN	E	6	11/12	0.95	0.11	70,74,80,81	0
2	MAN	D	6	11/12	0.96	0.12	64,75,82,85	0
2	MAN	E	4	11/12	0.96	0.10	62,72,79,80	0
2	BMA	D	3	11/12	0.96	0.09	59,63,73,76	0
2	NAG	D	2	14/15	0.96	0.12	52,62,72,79	0
2	BMA	F	3	11/12	0.96	0.10	38,45,47,49	0
2	MAN	F	6	11/12	0.96	0.11	43,48,51,51	0
2	MAN	F	4	11/12	0.96	0.08	45,50,53,62	0
2	NAG	E	2	14/15	0.96	0.11	57,72,80,82	0
2	NAG	C	2	14/15	0.97	0.13	31,49,62,66	0
2	NAG	F	5	14/15	0.97	0.11	38,45,50,51	0
2	BMA	E	3	11/12	0.97	0.09	68,71,76,76	0
2	NAG	F	7	14/15	0.97	0.11	44,48,55,56	0
2	BMA	C	3	11/12	0.97	0.10	46,52,56,64	0
2	MAN	D	4	11/12	0.97	0.14	53,65,74,80	0
2	NAG	F	2	14/15	0.98	0.12	37,43,48,49	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
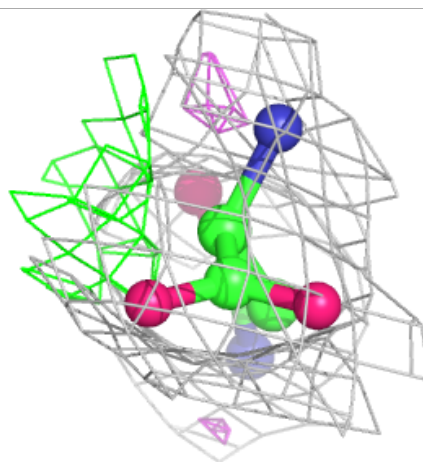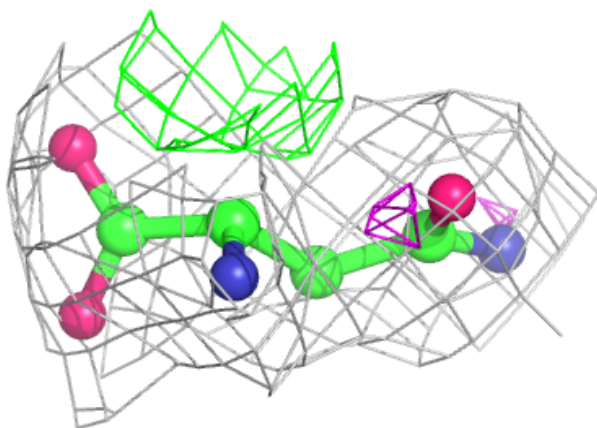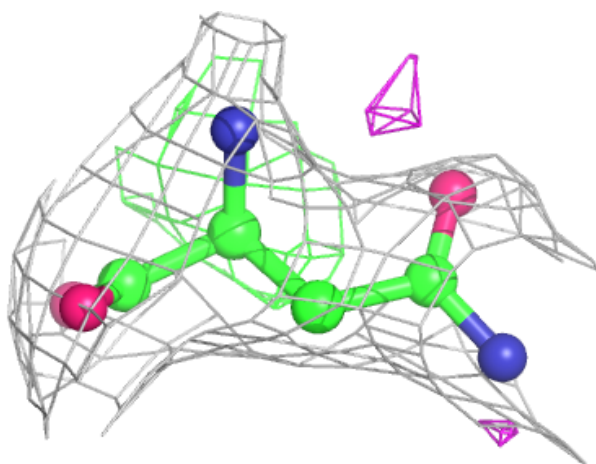mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
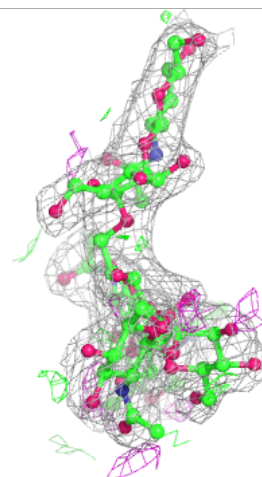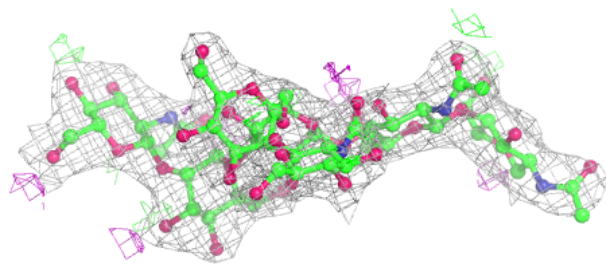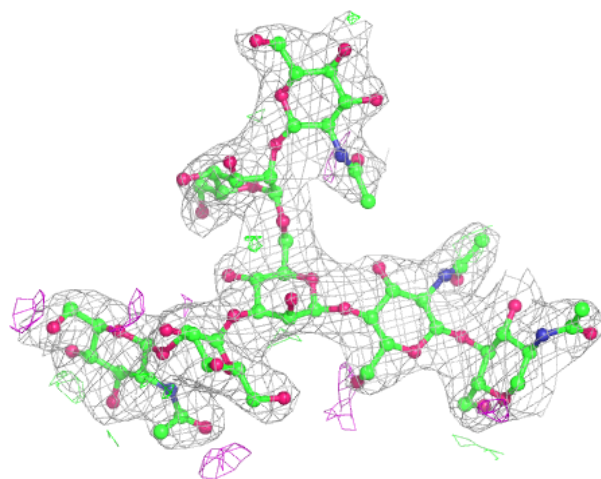
Electron density around Chain F:

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

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ASN	G	601	9/9	0.70	0.27	92,101,104,105	0
5	SO4	A	613	5/5	0.84	0.20	131,134,137,138	0
3	ASN	H	601	9/9	0.84	0.18	69,87,100,100	0
3	ASN	A	601	9/9	0.84	0.20	77,90,104,104	0
5	SO4	H	613	5/5	0.85	0.19	157,158,164,169	0
3	ASN	B	601	9/9	0.87	0.20	75,85,106,107	0
5	SO4	G	610	5/5	0.89	0.22	177,177,180,181	0
5	SO4	A	610	5/5	0.89	0.17	86,94,95,105	0
5	SO4	A	612	5/5	0.89	0.15	103,105,109,111	0
5	SO4	H	609	5/5	0.92	0.18	60,82,87,94	0
5	SO4	B	610	5/5	0.92	0.13	111,112,113,116	0
5	SO4	A	611	5/5	0.92	0.22	98,103,106,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
5	SO4	H	610	5/5	0.93	0.12	85,86,93,96	0
5	SO4	H	612	5/5	0.93	0.26	91,95,98,101	0
4	GDP	B	609	28/28	0.95	0.13	38,54,73,75	0
5	SO4	H	611	5/5	0.96	0.11	80,81,86,88	0
5	SO4	G	609	5/5	0.97	0.13	77,78,84,87	0
4	GDP	A	609	28/28	0.97	0.13	38,53,63,73	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.
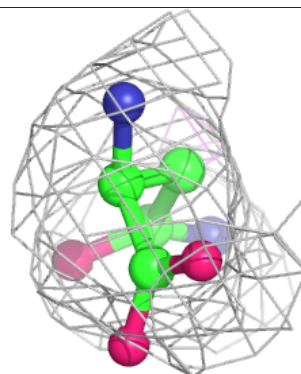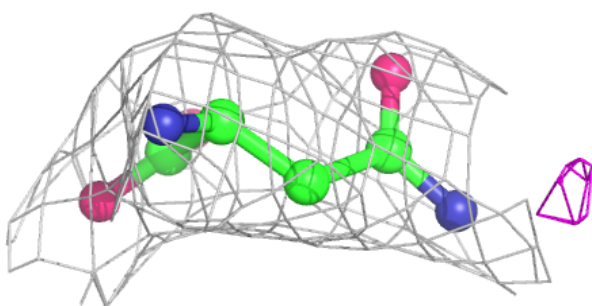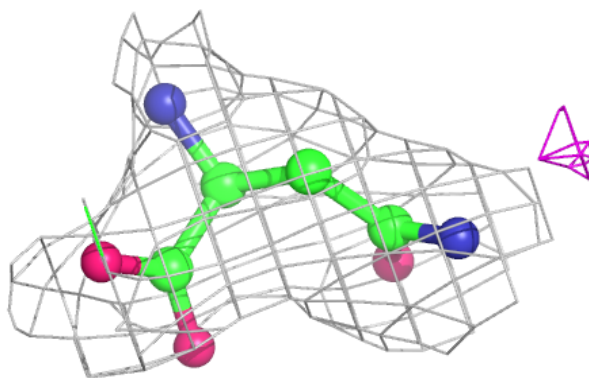
Electron density around ASN G 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
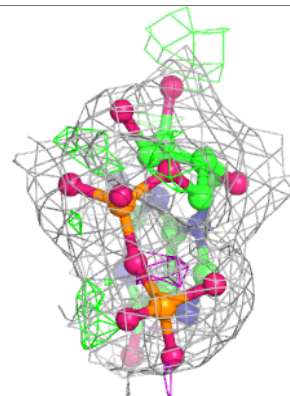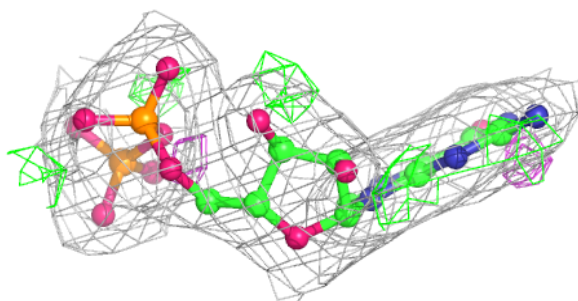mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
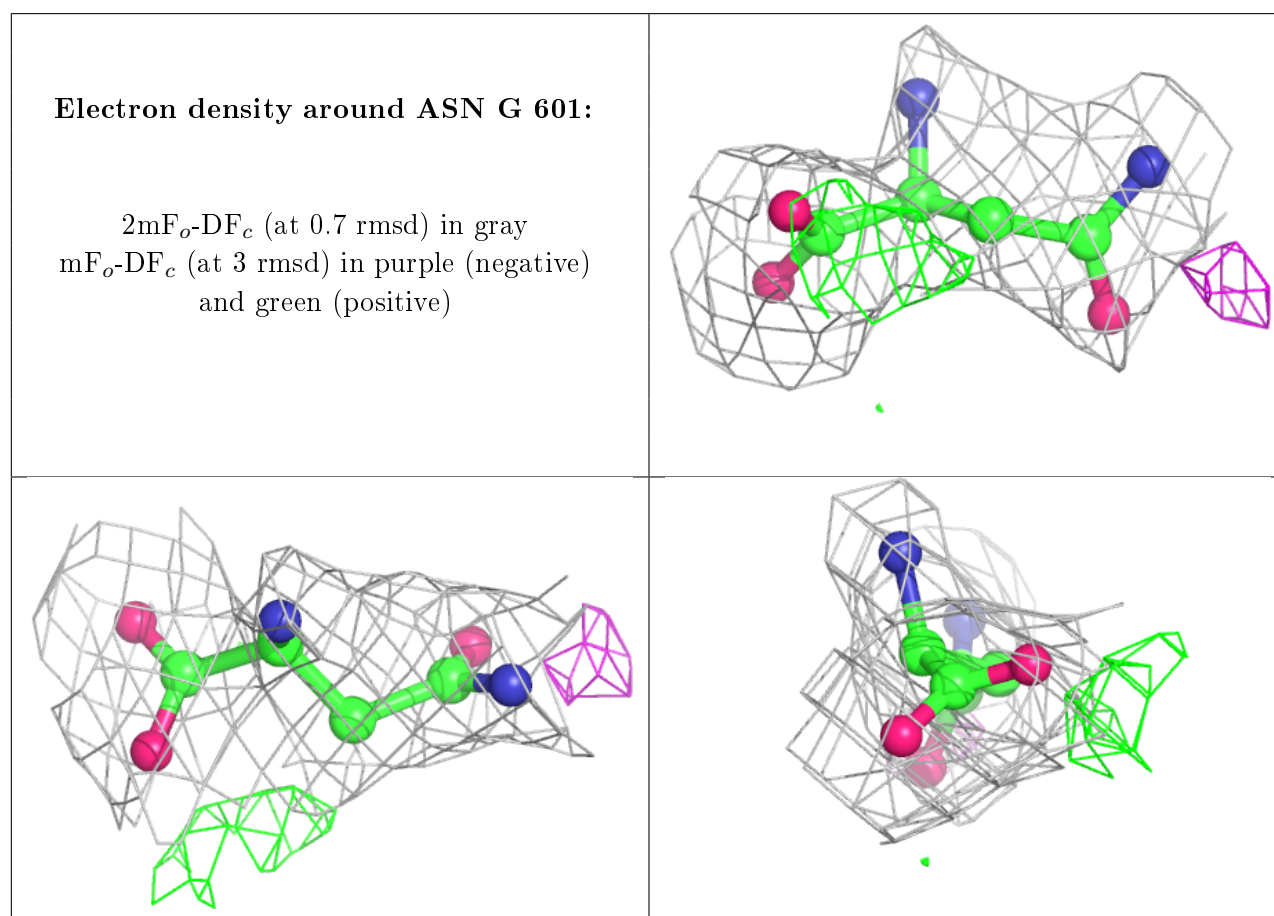
Electron density around ASN H 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
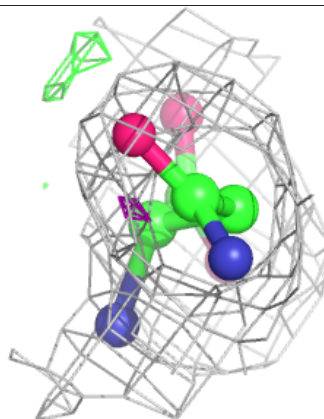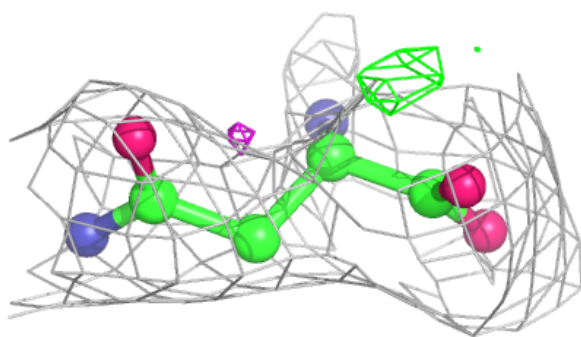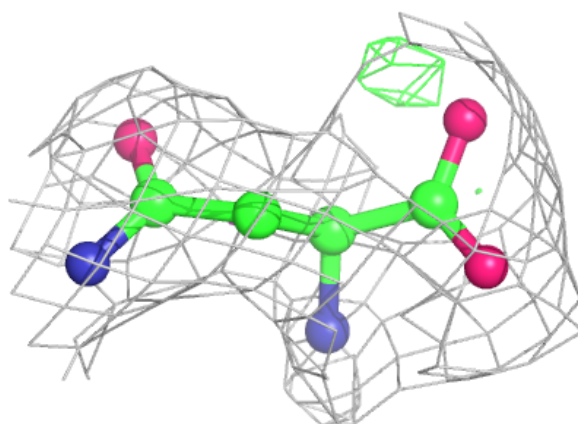
Electron density around ASN A 601:

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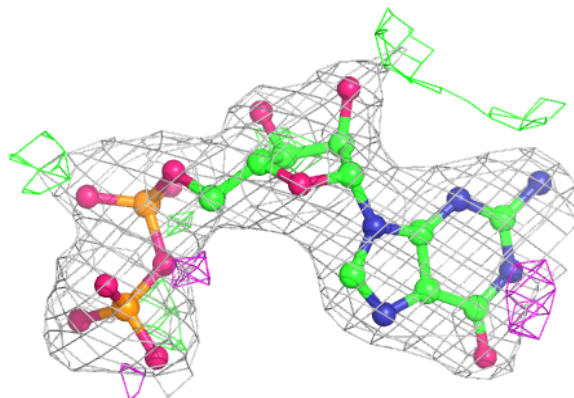$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ASN B 601:

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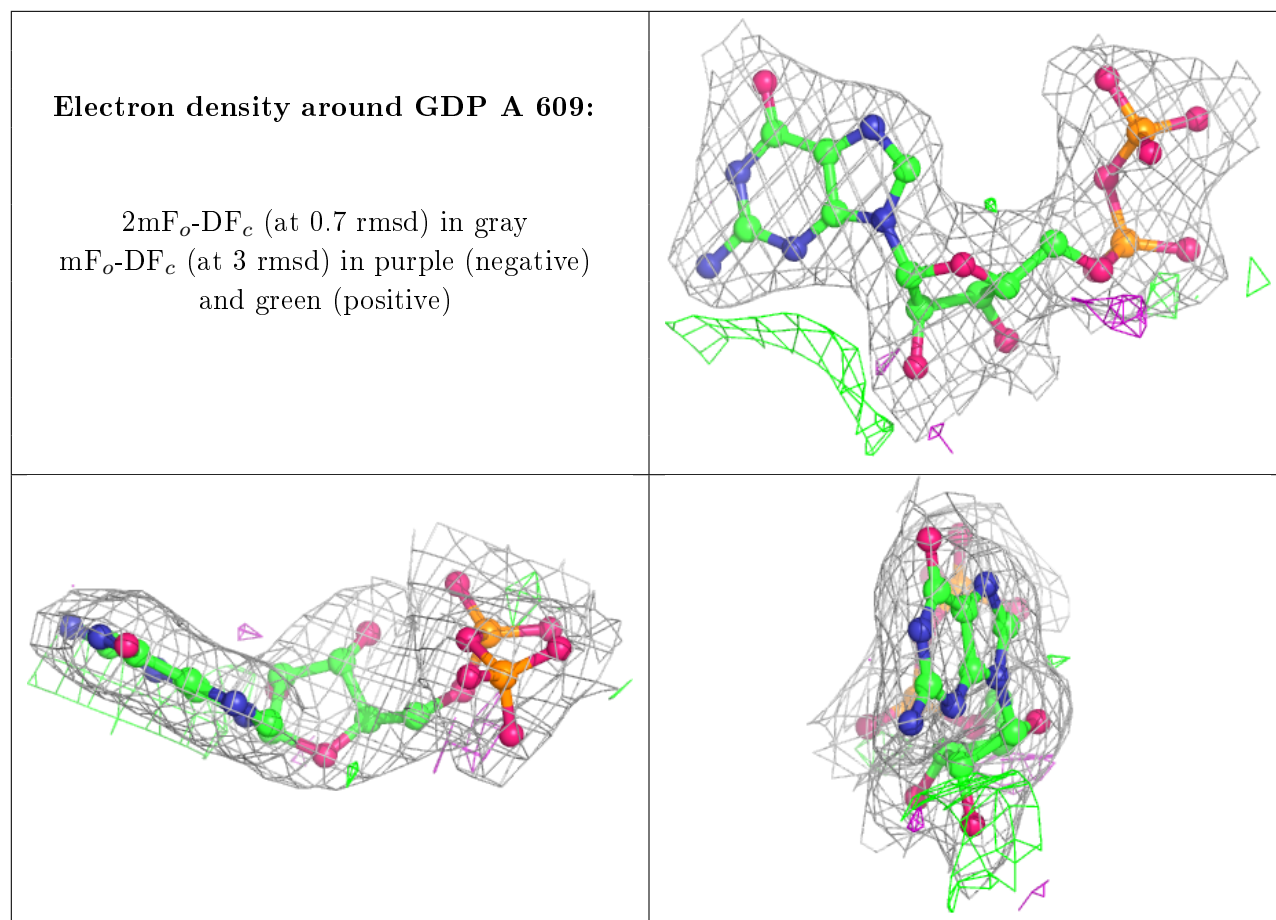and green (positive)

Electron density around GDP B 609:

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

Electron density around GDP A 609:

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

6.5 Other polymers (i)

There are no such residues in this entry.