Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 05:21 PM JST

PDB ID	:	5GMG
Title	:	Crystal structure of monkey TLR7 in complex with loxoribine and polyU
Authors	:	Zhang, Z.; Ohto, U.; Shimizu, T.
Deposited on	:	2016-07-14
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

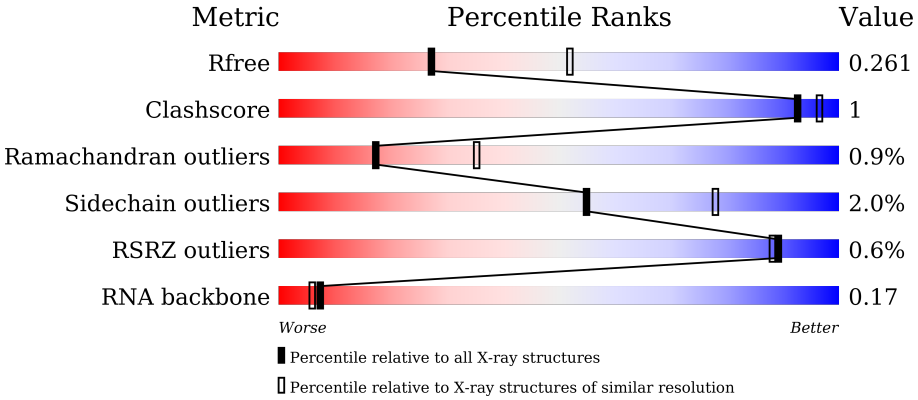
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	817	87% 6% 7%
1	B	817	% 87% 6% 7%
2	C	4	75% 25%
2	D	4	100%

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Mol	Chain	Length	Quality of chain
3	E	2	100%
3	F	2	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12680 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 Toll-like receptor 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	762	6166	3952	1050	1134	30	0	0	0
1	B	762	6160	3949	1047	1134	30	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP B3Y653
A	24	SER	-	expression tag	UNP B3Y653
A	25	PRO	-	expression tag	UNP B3Y653
A	26	TRP	-	expression tag	UNP B3Y653
A	167	GLN	ASN	engineered mutation	UNP B3Y653
A	389	GLN	ASN	engineered mutation	UNP B3Y653
A	488	GLN	ASN	engineered mutation	UNP B3Y653
A	799	GLN	ASN	engineered mutation	UNP B3Y653
B	23	ARG	-	expression tag	UNP B3Y653
B	24	SER	-	expression tag	UNP B3Y653
B	25	PRO	-	expression tag	UNP B3Y653
B	26	TRP	-	expression tag	UNP B3Y653
B	167	GLN	ASN	engineered mutation	UNP B3Y653
B	389	GLN	ASN	engineered mutation	UNP B3Y653
B	488	GLN	ASN	engineered mutation	UNP B3Y653
B	799	GLN	ASN	engineered mutation	UNP B3Y653

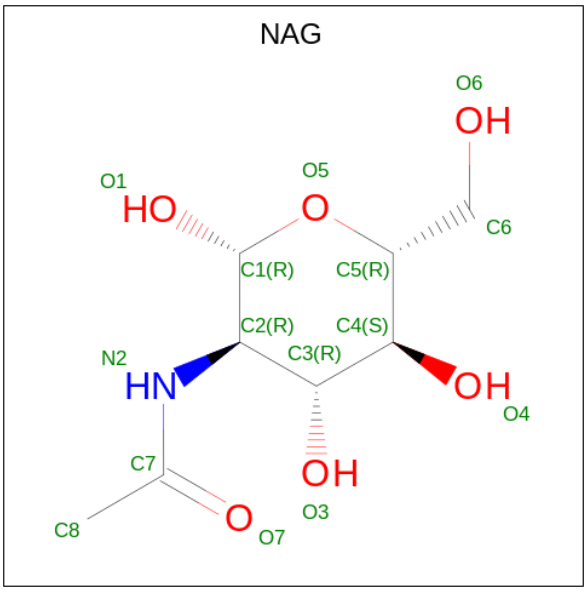
- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	4	64	27	6	27	4	0	0	0
2	D	4	64	27	6	27	4	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

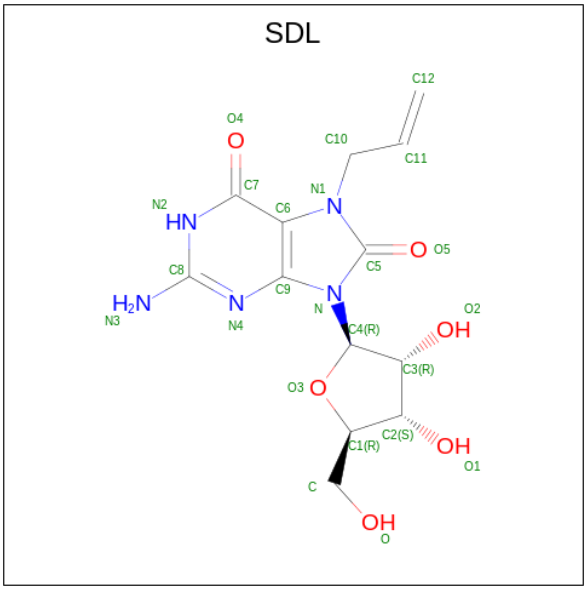
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	2	28	16	2	10	0	0	0
			Total	C	N	O			
3	F	2	28	16	2	10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



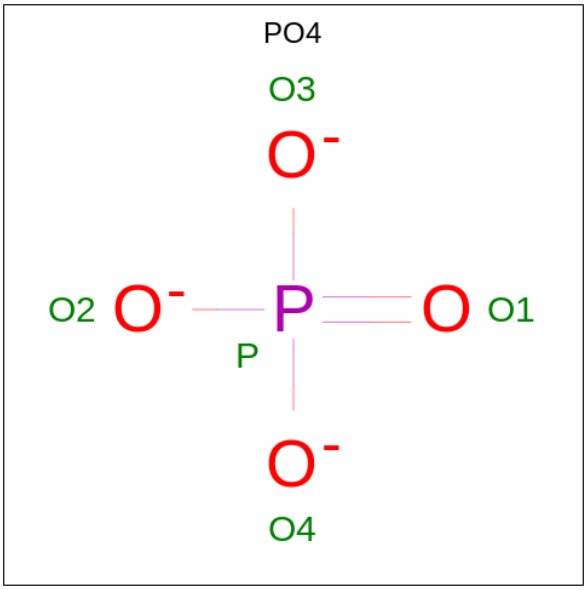
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	B	1	14	8	1	5	0	0
			Total	C	N	O		
4	B	1	14	8	1	5	0	0
			Total	C	N	O		
4	B	1	14	8	1	5	0	0

- Molecule 5 is 2-azanyl-9-[(2 {R},3 {R},4 {S},5 {R})-5-(hydroxymethyl)-3,4-bis(oxidanyl)oxolan-2-yl]-7-prop-2-enyl-1 {H}-purine-6,8-dione (three-letter code: SDL) (formula: $C_{13}H_{17}N_5O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	24	13	5	6	0	0
			Total	C	N	O		
5	B	1	24	13	5	6	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
6	B	1	5	4	1	0	0

- Molecule 7 is water.

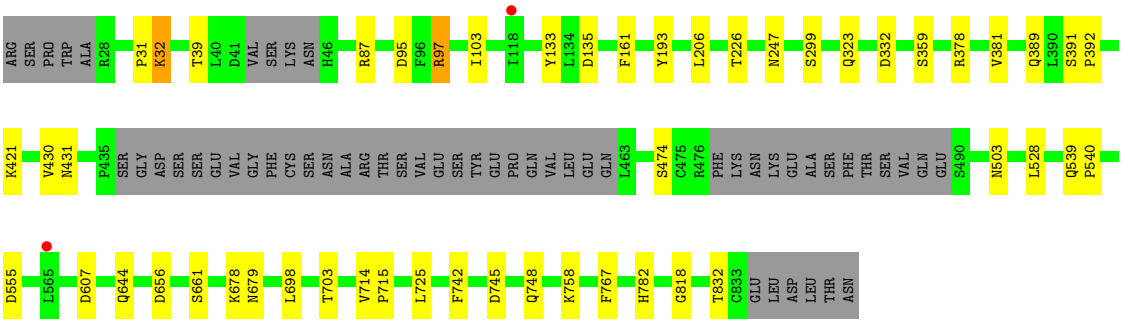
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	16	16	16	0	0
			Total	O		
7	B	17	17	17	0	0

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.

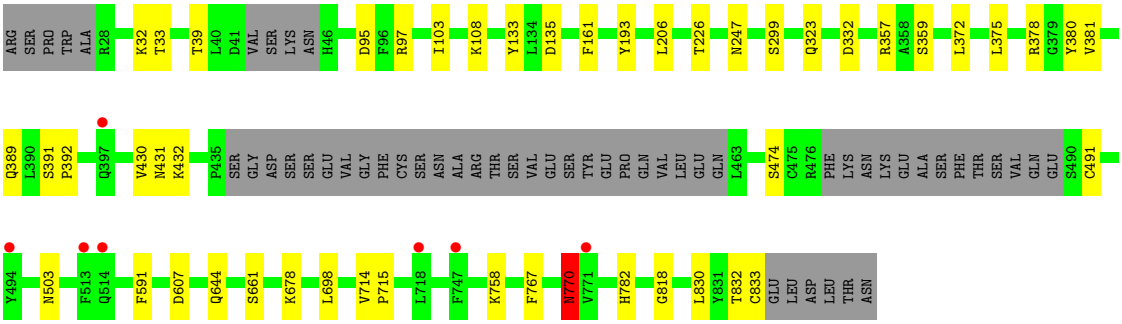
• Molecule 1: Toll-like receptor 7

Chain A:



• Molecule 1: Toll-like receptor 7

Chain B:



• Molecule 2: RNA (5'-R(P*UP*UP*UP*U)-3')

Chain C:

• Molecule 2: RNA (5'-R(P*UP*UP*UP*U)-3')

Chain D:

There are no outlier residues recorded for this chain.

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%

NAG1
NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.28Å 99.41Å 112.10Å 90.00° 98.58° 90.00°	Depositor
Resolution (Å)	50.01 – 2.60 48.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.5 (50.01-2.60) 93.6 (48.59-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.215 , 0.258 0.216 , 0.261	Depositor DCC
R_{free} test set	3088 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	64.0	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12680	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SDL, PO4, 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	0.61	0/6295	0.80	4/8530 (0.0%)
1	B	0.61	0/6289	0.79	4/8523 (0.0%)
2	C	0.50	0/69	0.78	0/105
2	D	0.42	0/69	0.93	0/105
All	All	0.61	0/12722	0.80	8/17263 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	378	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	378	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	B	378	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	378	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	833	CYS	CA-CB-SG	-5.64	103.85	114.00
1	B	770	ASN	CB-CA-C	-5.63	99.14	110.40
1	A	97	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	87	ARG	NE-CZ-NH1	5.07	122.83	120.30

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	6166	0	6206	21	0
1	B	6160	0	6195	17	0
2	C	64	0	30	0	0
2	D	64	0	30	0	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	A	42	0	39	1	0
4	B	42	0	39	1	0
5	B	48	0	0	0	0
6	B	5	0	0	0	0
7	A	16	0	0	2	0
7	B	17	0	0	0	0
All	All	12680	0	12589	37	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 1.

All (37) 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:679:ASN:HB2	1:A:703:THR:HB	1.59	0.85
1:A:679:ASN:CB	1:A:703:THR:HB	2.24	0.66
1:B:431:ASN:HB2	1:B:503:ASN:HD21	1.69	0.58
1:A:299:SER:HA	1:A:323:GLN:O	2.04	0.58
1:B:299:SER:HA	1:B:323:GLN:O	2.05	0.57
1:A:431:ASN:HB2	1:A:503:ASN:HD21	1.70	0.54
1:B:247:ASN:OD1	1:B:247:ASN:N	2.43	0.52
1:A:206:LEU:O	1:A:226:THR:HG23	2.10	0.52
1:A:555:ASP:OD2	1:B:432:LYS:NZ	2.43	0.52
1:A:247:ASN:N	1:A:247:ASN:OD1	2.44	0.50
1:B:206:LEU:O	1:B:226:THR:HG23	2.09	0.50
1:B:431:ASN:CB	1:B:503:ASN:HD21	2.24	0.50
1:B:770:ASN:H	1:B:770:ASN:HD22	1.58	0.50
1:A:656:ASP:HB2	4:A:904:NAG:H81	1.94	0.49
1:A:31:PRO:HA	1:A:32:LYS:CB	2.42	0.49
1:A:421:LYS:NZ	7:A:1004:HOH:O	2.45	0.49
1:B:714:VAL:HB	1:B:715:PRO:HD2	1.93	0.49
1:A:431:ASN:CB	1:A:503:ASN:HD21	2.26	0.49
1:B:95:ASP:OD1	1:B:97:ARG:HD3	2.14	0.48
1:A:714:VAL:HB	1:A:715:PRO:HD2	1.96	0.48
1:A:95:ASP:OD1	1:A:97:ARG:HD3	2.15	0.47
1:A:725:LEU:O	1:A:748:GLN:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ASP:HA	1:B:133:TYR:HB2	1.99	0.45
1:A:528:LEU:HA	7:A:1003:HOH:O	2.16	0.45
1:A:95:ASP:HA	1:A:133:TYR:HB2	1.99	0.44
1:B:359:SER:HB2	1:B:389:GLN:NE2	2.34	0.43
1:A:161:PHE:HA	1:A:193:TYR:CE1	2.54	0.43
1:B:372:LEU:HD21	1:B:375:LEU:HB2	2.00	0.43
1:A:359:SER:HB2	1:A:389:GLN:NE2	2.34	0.42
1:B:491:CYS:HB3	4:B:906:NAG:H81	2.02	0.42
1:B:161:PHE:HA	1:B:193:TYR:CE1	2.54	0.42
1:B:391:SER:N	1:B:392:PRO:CD	2.84	0.41
1:B:97:ARG:NH2	1:B:474:SER:O	2.54	0.41
1:A:97:ARG:NH2	1:A:474:SER:O	2.53	0.41
1:A:391:SER:N	1:A:392:PRO:CD	2.84	0.41
1:A:539:GLN:N	1:A:540:PRO:CD	2.84	0.41
1:B:357:ARG:HD2	1:B:380:TYR:CE1	2.57	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	754/817 (92%)	690 (92%)	58 (8%)	6 (1%)	19	39
1	B	754/817 (92%)	683 (91%)	64 (8%)	7 (1%)	17	35
All	All	1508/1634 (92%)	1373 (91%)	122 (8%)	13 (1%)	17	35

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	818	GLY
1	B	818	GLY
1	A	32	LYS

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Mol	Chain	Res	Type
1	A	332	ASP
1	B	332	ASP
1	B	32	LYS
1	B	832	THR
1	A	381	VAL
1	B	381	VAL
1	B	591	PHE
1	A	742	PHE
1	A	430	VAL
1	B	430	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	715/768 (93%)	702 (98%)	13 (2%)	59	80
1	B	714/768 (93%)	699 (98%)	15 (2%)	53	77
All	All	1429/1536 (93%)	1401 (98%)	28 (2%)	55	78

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	103	ILE
1	A	135	ASP
1	A	607	ASP
1	A	644	GLN
1	A	661	SER
1	A	678	LYS
1	A	698	LEU
1	A	745	ASP
1	A	758	LYS
1	A	767	PHE
1	A	782	HIS
1	A	832	THR

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Mol	Chain	Res	Type
1	B	33	THR
1	B	39	THR
1	B	103	ILE
1	B	108	LYS
1	B	135	ASP
1	B	607	ASP
1	B	644	GLN
1	B	661	SER
1	B	678	LYS
1	B	698	LEU
1	B	758	LYS
1	B	767	PHE
1	B	770	ASN
1	B	782	HIS
1	B	830	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	503	ASN
1	A	581	GLN
1	A	800	HIS
1	A	820	HIS
1	B	90	HIS
1	B	503	ASN
1	B	581	GLN
1	B	734	GLN
1	B	770	ASN
1	B	800	HIS
1	B	820	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	2/4 (50%)	0	1 (50%)
2	D	2/4 (50%)	0	0
All	All	4/8 (50%)	0	1 (25%)

There are no RNA backbone outliers to report.

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	3	U

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)

4 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	$\#\|Z\| > 2$
3	NAG	E	1	1,3	14,14,15	0.52	0	17,19,21	1.67	4 (23%)
3	NAG	E	2	3	14,14,15	0.59	0	17,19,21	1.78	4 (23%)
3	NAG	F	1	1,3	14,14,15	0.50	0	17,19,21	1.56	3 (17%)
3	NAG	F	2	3	14,14,15	0.92	1 (7%)	17,19,21	1.82	4 (23%)

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
3	NAG	E	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	C1-C2	2.20	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2	NAG	C1-O5-C5	4.37	118.11	112.19
3	F	2	NAG	C4-C3-C2	3.88	116.71	111.02
3	F	1	NAG	O5-C5-C6	3.79	113.14	107.20
3	F	2	NAG	C1-C2-N2	3.25	116.04	110.49
3	F	2	NAG	O3-C3-C2	-2.91	103.45	109.47
3	E	1	NAG	O5-C5-C6	-2.70	102.97	107.20
3	E	2	NAG	C3-C4-C5	-2.62	105.57	110.24
3	F	2	NAG	C2-N2-C7	2.61	126.62	122.90
3	F	1	NAG	O7-C7-N2	2.60	126.72	121.95
3	E	2	NAG	O4-C4-C5	2.57	115.68	109.30
3	F	1	NAG	O5-C1-C2	-2.34	107.59	111.29
3	E	1	NAG	O4-C4-C5	2.27	114.94	109.30
3	E	1	NAG	C4-C3-C2	2.22	114.27	111.02
3	E	1	NAG	C3-C4-C5	-2.06	106.56	110.24
3	E	2	NAG	O5-C1-C2	-2.05	108.05	111.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

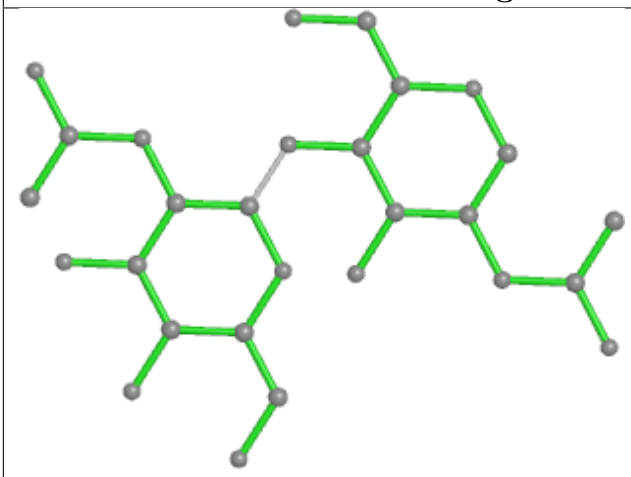
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6

There are no ring outliers.

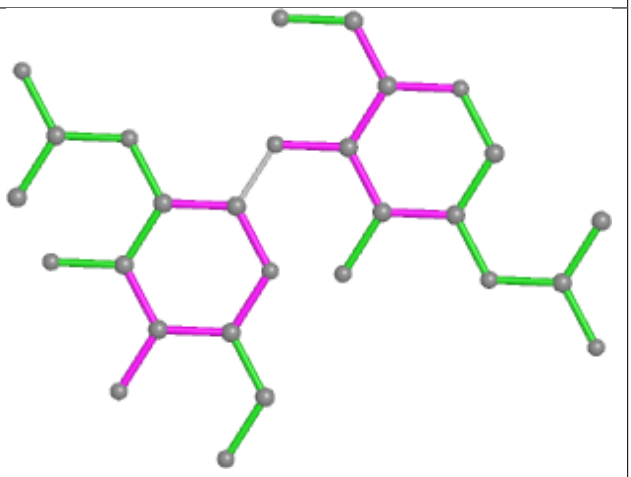
No monomer is involved in short contacts.

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

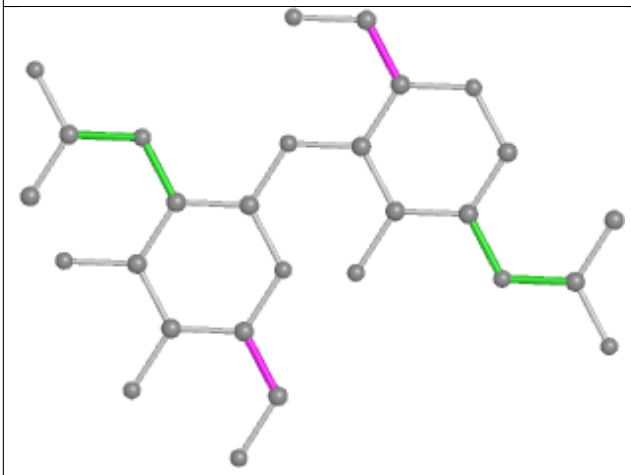
Oligosaccharide Chain E



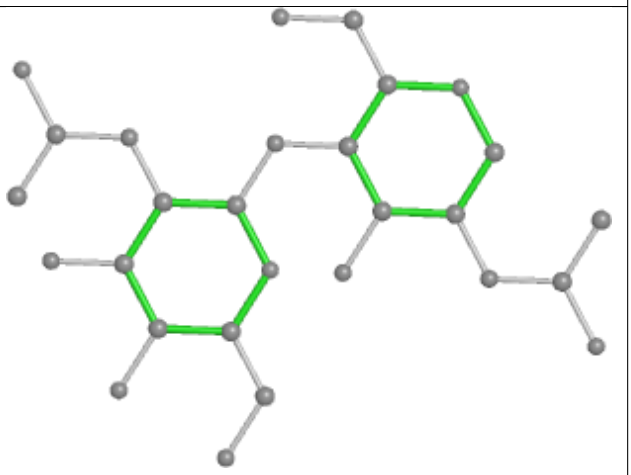
Bond lengths



Bond angles

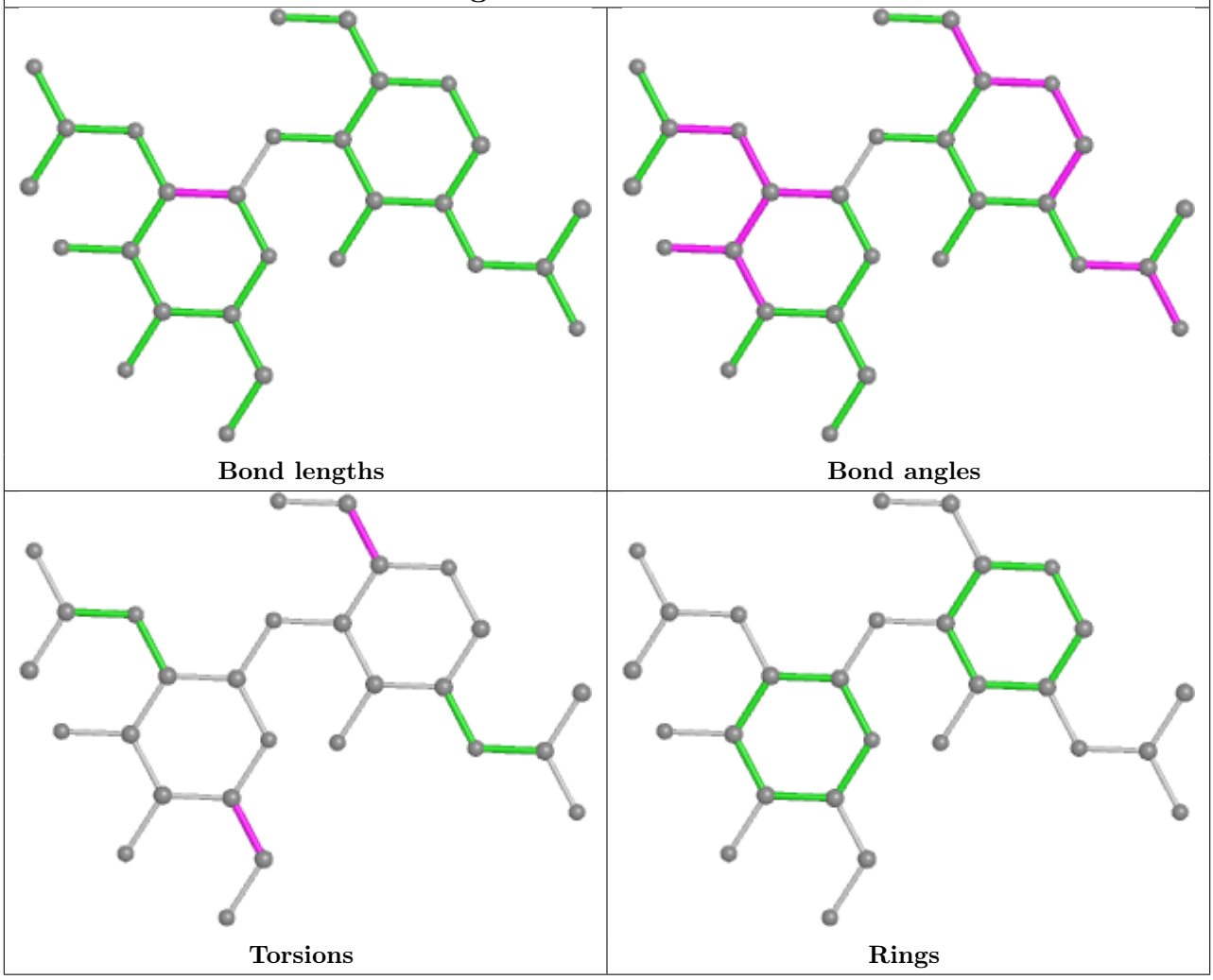


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	905	1	14,14,15	0.45	0	17,19,21	1.83	6 (35%)
5	SDL	B	902	-	26,26,26	1.74	6 (23%)	35,39,39	3.40	13 (37%)
4	NAG	B	906	1	14,14,15	0.51	0	17,19,21	1.33	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SDL	B	901	-	26,26,26	1.71	7 (26%)	35,39,39	3.44	11 (31%)
4	NAG	B	903	1	14,14,15	0.50	0	17,19,21	2.78	5 (29%)
6	PO4	B	908	-	4,4,4	0.68	0	6,6,6	0.91	0
4	NAG	A	904	1	14,14,15	0.62	0	17,19,21	2.13	5 (29%)
4	NAG	A	901	1	14,14,15	0.89	1 (7%)	17,19,21	1.62	4 (23%)
4	NAG	B	907	1	14,14,15	0.75	1 (7%)	17,19,21	2.30	5 (29%)

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	A	905	1	-	1/6/23/26	0/1/1/1
5	SDL	B	902	-	-	1/9/25/25	0/3/3/3
4	NAG	B	906	1	-	0/6/23/26	0/1/1/1
5	SDL	B	901	-	-	0/9/25/25	0/3/3/3
4	NAG	B	903	1	-	0/6/23/26	0/1/1/1
4	NAG	A	904	1	-	3/6/23/26	0/1/1/1
4	NAG	A	901	1	-	2/6/23/26	0/1/1/1
4	NAG	B	907	1	-	2/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	902	SDL	C5-N	-3.83	1.34	1.40
5	B	901	SDL	C5-N	-3.69	1.34	1.40
5	B	901	SDL	O5-C5	3.43	1.28	1.22
5	B	902	SDL	O5-C5	3.36	1.28	1.22
5	B	902	SDL	C9-N	-3.09	1.33	1.39
5	B	902	SDL	C5-N1	-3.08	1.33	1.39
5	B	901	SDL	C5-N1	-3.04	1.33	1.39
5	B	901	SDL	C6-C9	2.99	1.47	1.38
5	B	902	SDL	C6-C9	2.75	1.47	1.38
5	B	901	SDL	C9-N	-2.72	1.34	1.39
5	B	901	SDL	C6-N1	-2.64	1.34	1.39
5	B	902	SDL	C6-N1	-2.44	1.34	1.39
4	B	907	NAG	O4-C4	2.35	1.48	1.43
5	B	901	SDL	C6-C7	2.09	1.48	1.43
4	A	901	NAG	C1-C2	2.09	1.55	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	901	SDL	N-C5-N1	13.49	116.55	106.86
5	B	902	SDL	N-C5-N1	11.54	115.15	106.86
5	B	902	SDL	N-C9-N4	9.65	136.84	125.81
5	B	901	SDL	N-C9-N4	9.24	136.37	125.81
4	B	903	NAG	C1-O5-C5	9.22	124.69	112.19
4	A	904	NAG	C1-O5-C5	6.16	120.54	112.19
4	B	907	NAG	C1-O5-C5	5.77	120.01	112.19
5	B	901	SDL	C6-C9-N4	-5.39	117.86	128.13
5	B	902	SDL	O3-C4-N	-5.15	101.08	108.72
5	B	902	SDL	C9-C6-N1	5.15	109.49	104.91
5	B	901	SDL	C8-N4-C9	5.10	121.39	112.30
5	B	902	SDL	C6-C9-N4	-5.09	118.42	128.13
5	B	902	SDL	C8-N4-C9	4.84	120.92	112.30
5	B	901	SDL	C9-C6-N1	4.58	108.99	104.91
4	B	907	NAG	C3-C4-C5	-4.50	102.22	110.24
4	B	903	NAG	C2-N2-C7	4.41	129.19	122.90
4	A	905	NAG	C1-O5-C5	4.39	118.13	112.19
5	B	902	SDL	C6-C7-N2	3.54	117.22	110.99
4	B	906	NAG	C1-O5-C5	3.54	116.98	112.19
4	A	901	NAG	C3-C4-C5	-3.49	104.01	110.24
4	B	907	NAG	O4-C4-C5	3.45	117.87	109.30
5	B	901	SDL	O3-C4-N	-3.37	103.72	108.72
4	B	907	NAG	O5-C1-C2	-3.30	106.08	111.29
4	A	901	NAG	C1-O5-C5	3.28	116.63	112.19
5	B	902	SDL	C2-C3-C4	-3.13	95.49	101.43
5	B	901	SDL	C5-N-C9	-3.10	105.30	109.40
5	B	901	SDL	C10-N1-C6	3.05	129.88	125.28
4	A	904	NAG	C4-C3-C2	-3.02	106.60	111.02
5	B	902	SDL	O2-C3-C4	3.00	120.04	110.02
5	B	902	SDL	C3-C4-N	2.85	119.73	115.94
4	A	901	NAG	O4-C4-C5	2.82	116.29	109.30
4	B	903	NAG	O7-C7-N2	2.73	126.97	121.95
5	B	901	SDL	C6-C7-N2	2.70	115.74	110.99
4	A	905	NAG	C6-C5-C4	-2.62	106.86	113.00
4	A	904	NAG	O7-C7-N2	2.59	126.71	121.95
5	B	902	SDL	O4-C7-C6	-2.55	121.28	127.54
4	A	905	NAG	C1-C2-N2	-2.50	106.22	110.49
4	A	905	NAG	C8-C7-N2	-2.46	111.94	116.10
4	B	907	NAG	O5-C5-C6	-2.43	103.39	107.20
5	B	902	SDL	C10-N1-C6	2.36	128.83	125.28
4	A	901	NAG	C2-N2-C7	2.27	126.14	122.90
4	A	905	NAG	O5-C5-C4	2.26	116.32	110.83

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	906	NAG	O4-C4-C3	-2.25	105.15	110.35
4	A	904	NAG	O3-C3-C2	2.19	114.00	109.47
4	B	903	NAG	O7-C7-C8	-2.16	118.05	122.06
5	B	901	SDL	O5-C5-N	-2.16	122.62	126.54
5	B	901	SDL	C3-C4-N	2.15	118.80	115.94
4	B	903	NAG	O5-C1-C2	2.11	114.63	111.29
4	A	905	NAG	O7-C7-N2	2.10	125.82	121.95
5	B	902	SDL	C7-C6-C9	-2.09	118.32	122.62
4	A	904	NAG	C1-C2-N2	2.02	113.93	110.49

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	NAG	O5-C5-C6-O6
4	A	901	NAG	C4-C5-C6-O6
4	B	907	NAG	C4-C5-C6-O6
4	A	905	NAG	C4-C5-C6-O6
4	A	904	NAG	C1-C2-N2-C7
4	A	904	NAG	C3-C2-N2-C7
4	A	904	NAG	C4-C5-C6-O6
4	B	907	NAG	O5-C5-C6-O6
5	B	902	SDL	N1-C10-C11-C12

There are no ring outliers.

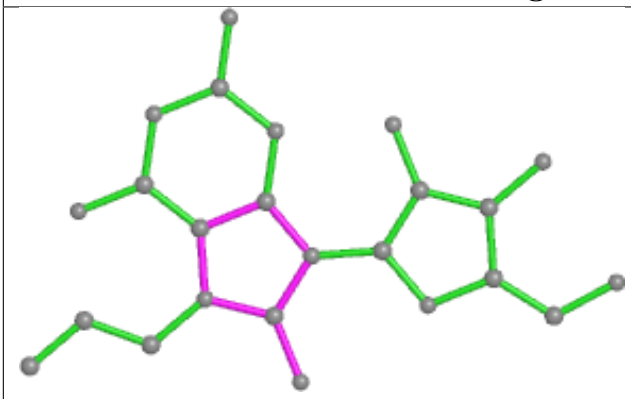
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	906	NAG	1	0
4	A	904	NAG	1	0

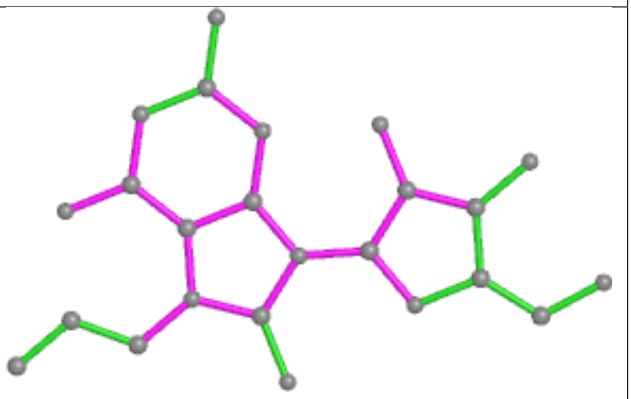
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

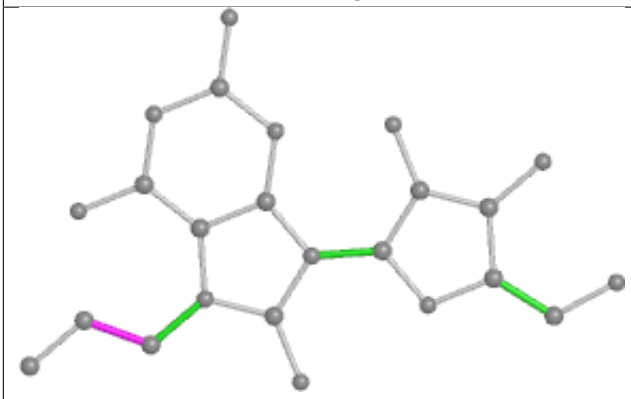
Ligand SDL B 902



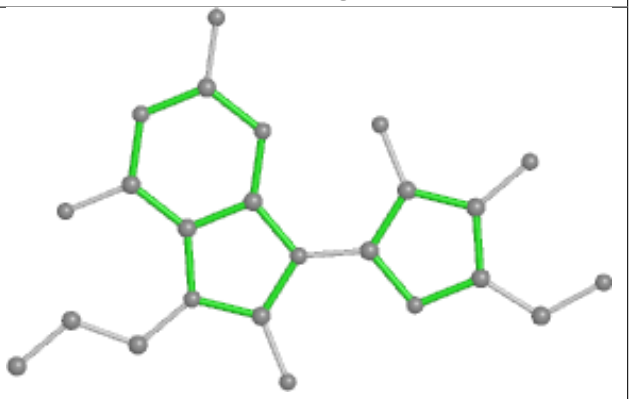
Bond lengths



Bond angles

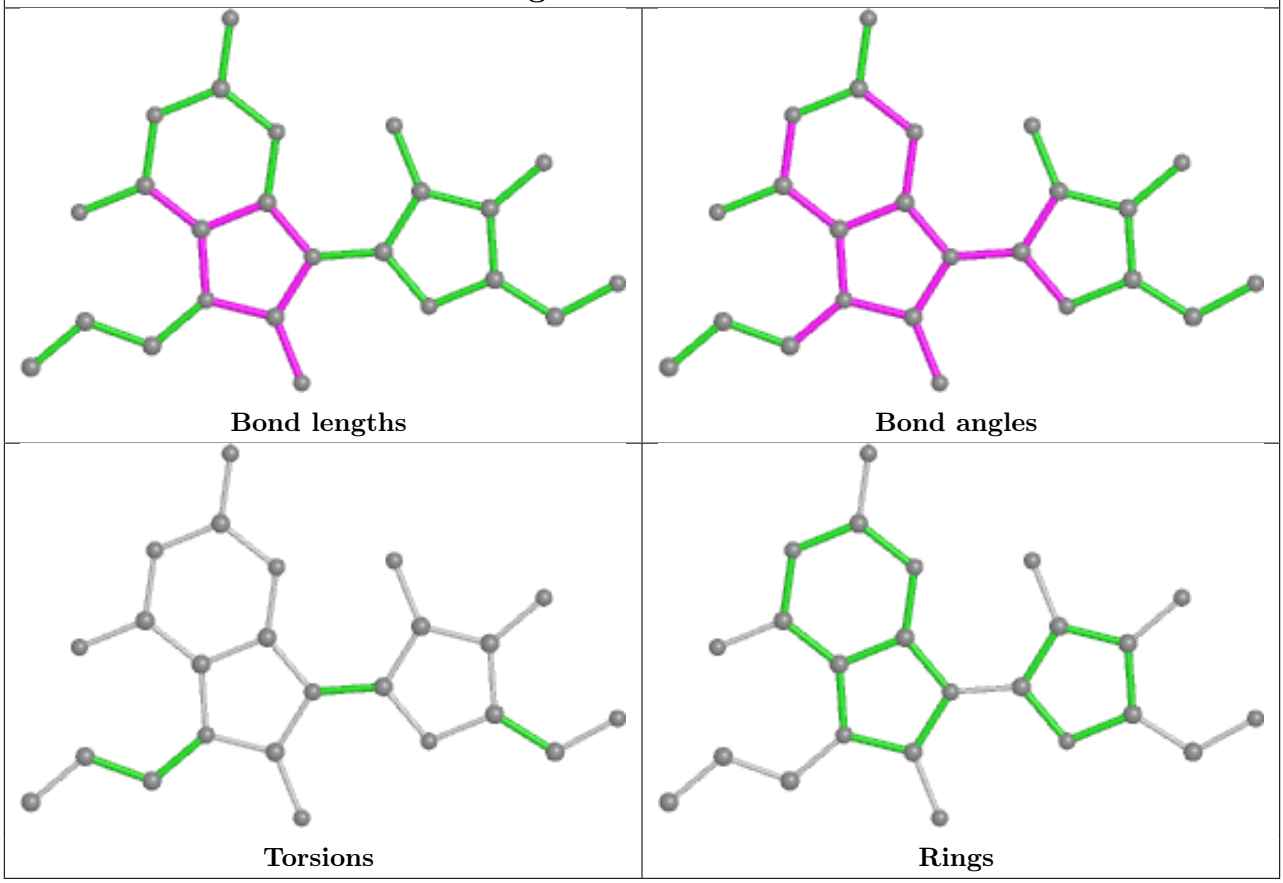


Torsions



Rings

Ligand SDL B 901



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	762/817 (93%)	-0.09	2 (0%)	94	93	37, 67, 97, 122	0
1	B	762/817 (93%)	-0.06	7 (0%)	84	82	40, 65, 94, 120	0
2	C	4/4 (100%)	-0.43	0	100	100	61, 72, 74, 82	0
2	D	4/4 (100%)	-0.44	0	100	100	54, 72, 73, 75	0
All	All	1532/1642 (93%)	-0.08	9 (0%)	89	88	37, 66, 96, 122	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	397	GLN	3.3
1	B	747	PHE	2.6
1	B	494	TYR	2.6
1	B	513	PHE	2.4
1	B	771	VAL	2.3
1	B	718	LEU	2.2
1	A	565	LEU	2.1
1	B	514	GLN	2.1
1	A	118	ILE	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)

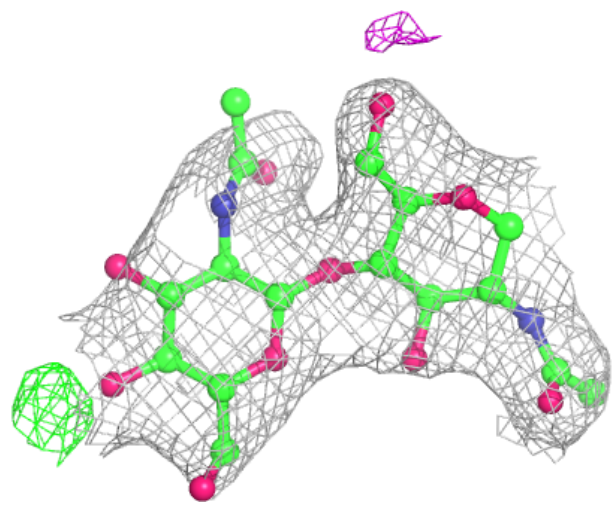
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

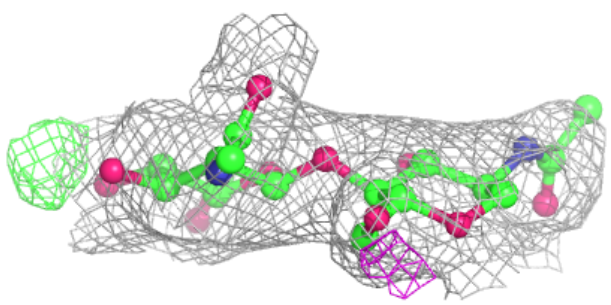
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	E	2	14/15	0.86	0.16	88,99,102,110	0
3	NAG	F	2	14/15	0.90	0.16	69,78,84,84	0
3	NAG	E	1	14/15	0.97	0.12	64,76,85,85	0
3	NAG	F	1	14/15	0.98	0.12	46,57,61,64	0

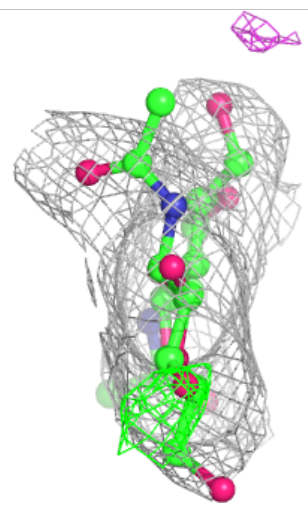
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

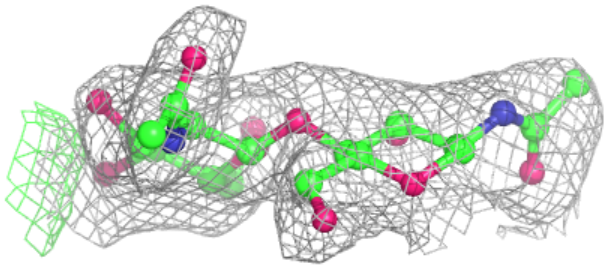


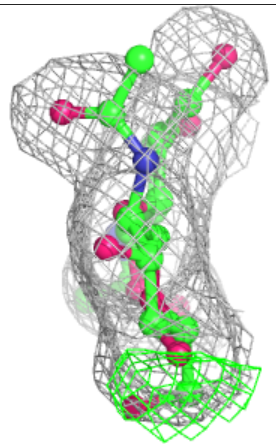




Electron density around Chain F:

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





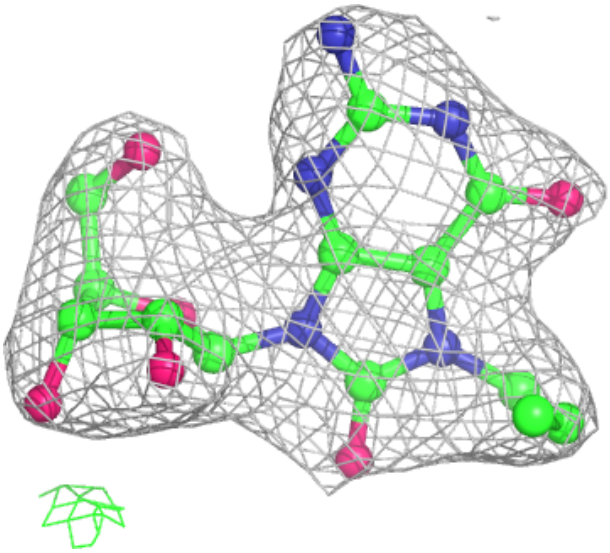
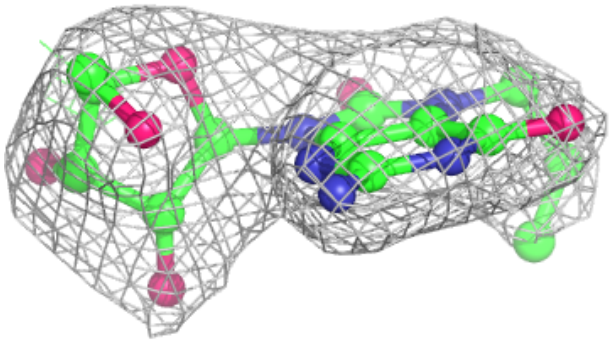
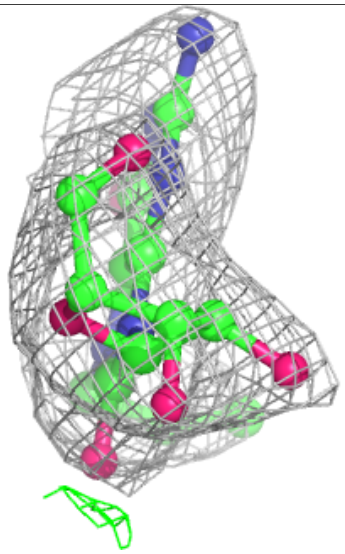
6.4 Ligands (i)

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
4	NAG	A	904	14/15	0.83	0.25	70,91,118,120	0
4	NAG	A	901	14/15	0.86	0.20	77,85,97,99	0
4	NAG	B	907	14/15	0.86	0.19	58,73,83,84	0
4	NAG	B	903	14/15	0.94	0.14	80,84,91,94	0
4	NAG	A	905	14/15	0.94	0.14	44,49,52,53	0
6	PO4	B	908	5/5	0.95	0.17	97,103,114,117	0
5	SDL	B	901	24/24	0.97	0.16	56,67,80,80	0
5	SDL	B	902	24/24	0.97	0.14	63,70,75,81	0
4	NAG	B	906	14/15	0.97	0.14	49,50,57,58	0

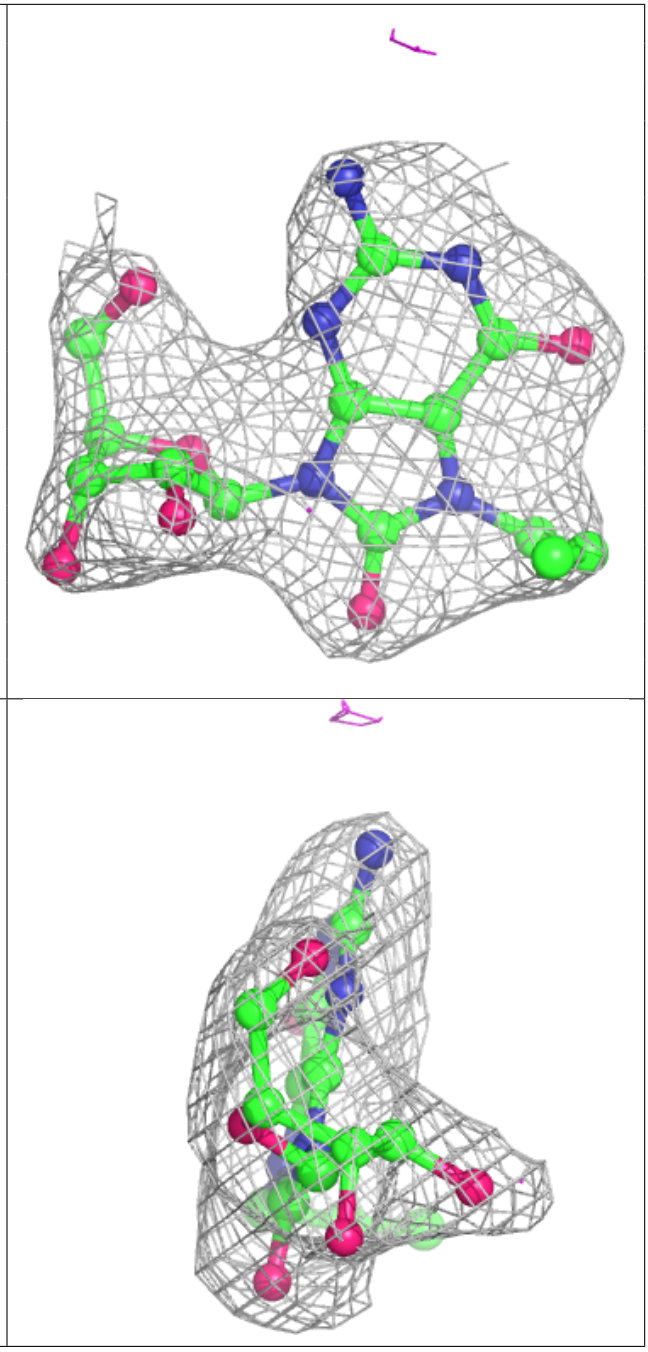
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

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 SDL B 901: 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 SDL B 902:

$2mF_o$-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.