wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2020 – 03:24 AM BST

PDB ID	:	6MUG
Title	:	Crystal Structure of HIV-1 B41 SOSIP.664 Prefusion Env Trimer Bound to Small Molecule HIV-1 Entry Inhibitor BMS-386150 in Complex with Human Antibodies 3H109L and 35O22 at 3.8 Angstrom
Authors	:	Lai, Y.-T.; Kwong, P.D.
Deposited on	:	2018-10-23
Resolution	:	2.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (1)) were used in the production of this report:

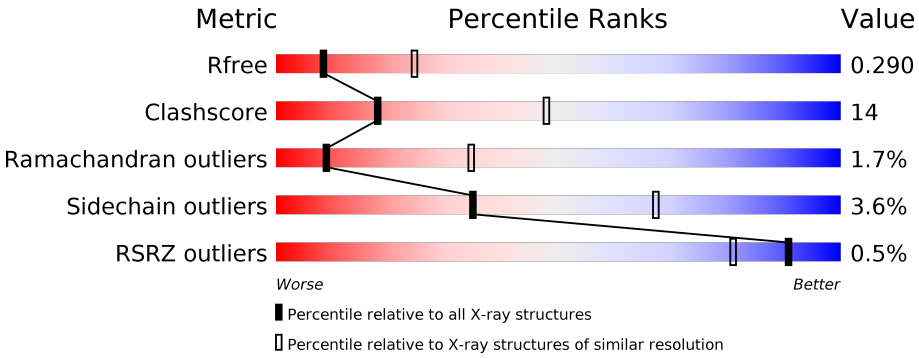
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	B	153	59% 19% 20%
2	D	134	61% 31%
3	E	114	3% 66% 32%
4	G	489	56% 28% 13%
5	H	244	64% 28% 7%
6	L	217	69% 26%

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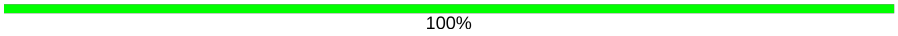
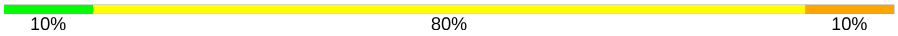
Mol	Chain	Length	Quality of chain
7	A	6	
8	C	2	
8	F	2	
9	I	10	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 9963 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	123	Total	C	N	O	S	0	0	0
			994	636	167	184	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP B3UEZ6
B	605	CYS	THR	engineered mutation	UNP B3UEZ6

- Molecule 2 is a protein called 35O22 scFv heavy chain portion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	128	Total	C	N	O	S	0	0	0
			994	628	169	192	5			

- Molecule 3 is a protein called 35O22 scFv light chain portion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	112	Total	C	N	O	S	0	0	0
			851	533	141	171	6			

- Molecule 4 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	424	Total	C	N	O	S	0	0	0
			3330	2101	587	616	26			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	conflict	UNP B3UES2
G	508	ARG	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	509	ARG	-	expression tag	UNP B3UES2
G	510	ARG	-	expression tag	UNP B3UES2
G	511	ARG	-	expression tag	UNP B3UES2
G	512	ARG	-	expression tag	UNP B3UES2
G	513	ARG	-	expression tag	UNP B3UES2

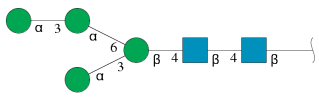
- Molecule 5 is a protein called 3H109L Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	227	Total	C	N	O	S	0	0	0
			1721	1096	279	340	6			

- Molecule 6 is a protein called 3H109L Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	211	Total	C	N	O	S	0	0	0
			1604	1009	276	312	7			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
7	A	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 8 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
8	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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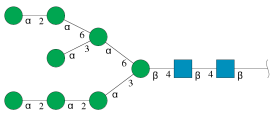
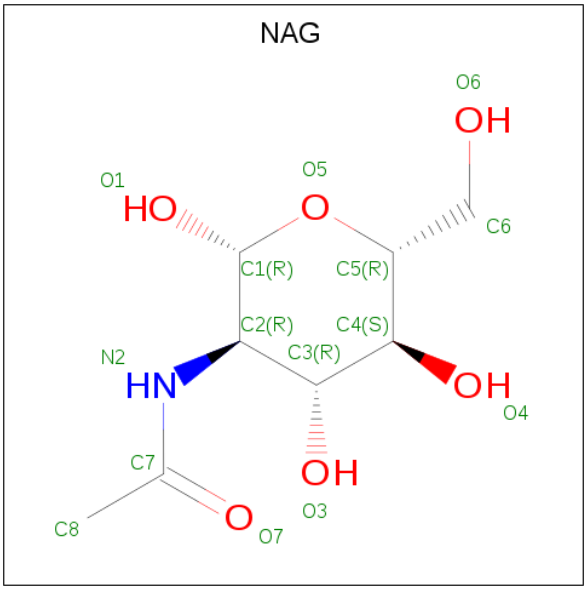
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	F	2	Total C N O 28 16 2 10	0	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
9	I	10	Total C N O 116 64 2 50	0	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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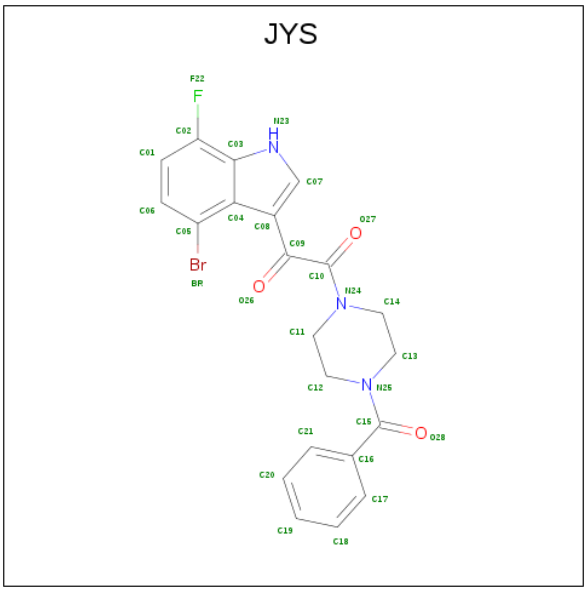
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	G	1	Total C N O 14 8 1 5	0	0
10	G	1	Total C N O 14 8 1 5	0	0
10	G	1	Total C N O 14 8 1 5	0	0
10	G	1	Total C N O 14 8 1 5	0	0
10	G	1	Total C N O 14 8 1 5	0	0
10	G	1	Total C N O 14 8 1 5	0	0
10	G	1	Total C N O 14 8 1 5	0	0
10	G	1	Total C N O 14 8 1 5	0	0
10	G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

- Molecule 11 is 1-[4-(benzenecarbonyl)piperazin-1-yl]-2-(4-bromo-7-fluoro-1H-indol-3-yl)ethane-1,2-dione (three-letter code: JYS) (formula: $C_{21}H_{17}BrFN_3O_3$) (labeled as "Ligand of Interest" by author).



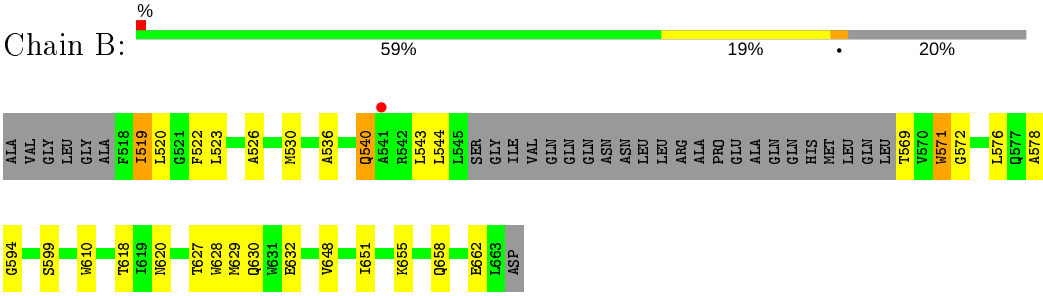
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	F	N	O		
11	G	1	29	1	21	1	3	3	0	0

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.

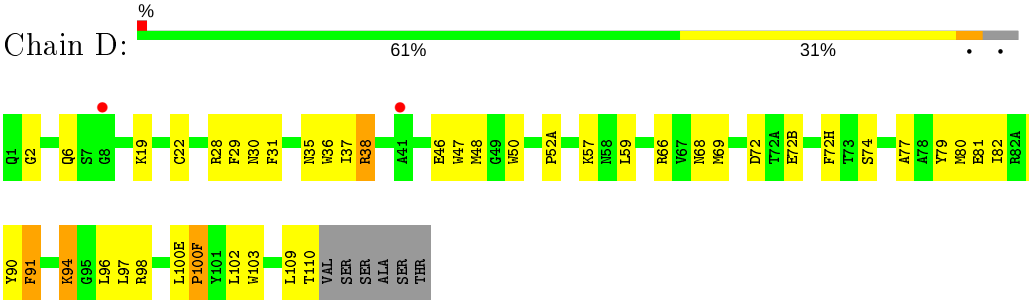
- Molecule 1: Envelope glycoprotein gp160

Chain B:



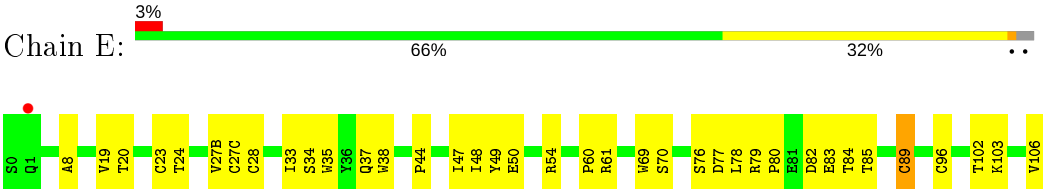
- Molecule 2: 35O22 scFv heavy chain portion

Chain D:



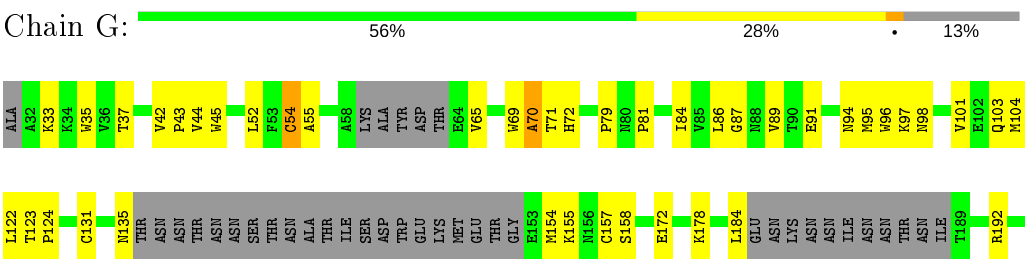
- Molecule 3: 35O22 scFv light chain portion

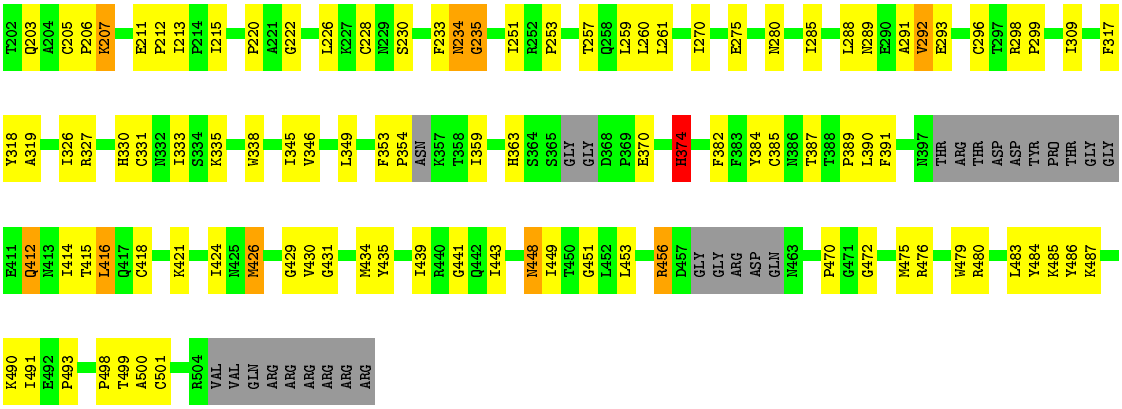
Chain E:



- Molecule 4: Envelope glycoprotein gp160

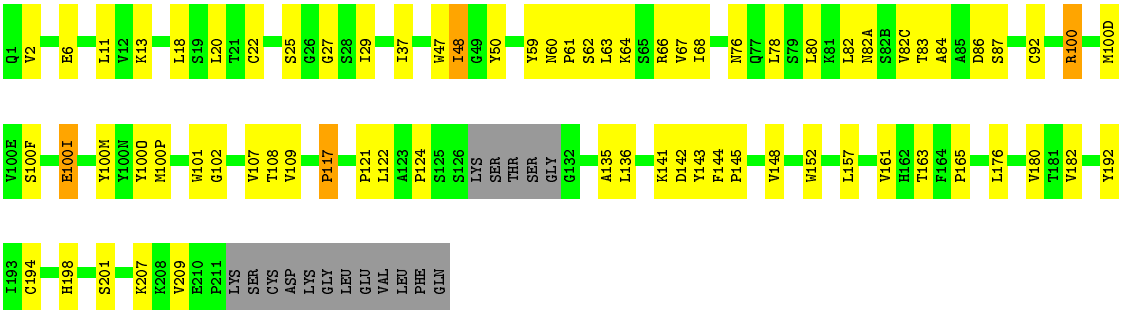
Chain G:





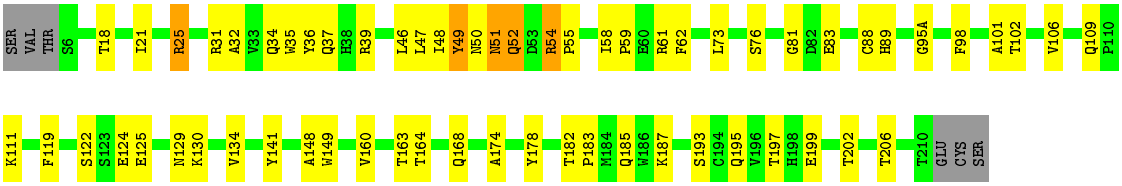
• Molecule 5: 3H109L Fab heavy chain

Chain H:



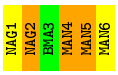
• Molecule 6: 3H109L Fab light chain

Chain L:



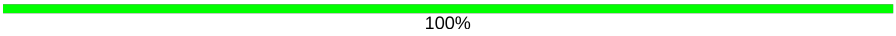
• Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:



• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

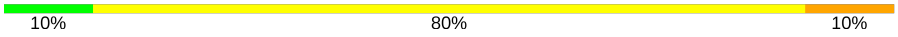


• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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 I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	132.76Å 132.76Å 313.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.88 – 2.95 41.88 – 2.75	Depositor EDS
% Data completeness (in resolution range)	30.2 (41.88-2.95) 24.4 (41.88-2.75)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.230 , 0.289 0.230 , 0.290	Depositor DCC
R_{free} test set	991 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , -11.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.095 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	9963	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: BMA, NAG, JYS, MAN

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	B	0.25	0/1013	0.43	0/1374
2	D	0.26	0/1021	0.49	0/1390
3	E	0.27	0/875	0.47	0/1195
4	G	0.29	0/3399	0.50	0/4617
5	H	0.27	0/1764	0.50	0/2405
6	L	0.27	0/1647	0.48	0/2247
All	All	0.27	0/9719	0.48	0/13228

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

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	B	994	0	980	27	0
2	D	994	0	953	28	0
3	E	851	0	801	20	0
4	G	3330	0	3268	108	0
5	H	1721	0	1690	48	0
6	L	1604	0	1553	47	0
7	A	72	0	61	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	28	0	25	0	0
8	F	28	0	25	1	0
9	I	116	0	97	2	0
10	B	28	0	26	0	0
10	G	168	0	156	2	0
11	G	29	0	0	2	0
All	All	9963	0	9635	265	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 14.

The worst 5 of 265 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)
4:G:335:LYS:HD2	4:G:412:GLN:HB3	1.65	0.77
4:G:52:LEU:H	4:G:103:GLN:HE22	1.32	0.75
6:L:34:GLN:HB2	6:L:89:HIS:HB3	1.69	0.74
1:B:651:ILE:HG13	1:B:655:LYS:HE3	1.68	0.74
1:B:523:LEU:HD12	1:B:540:GLN:HG2	1.69	0.74

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	B	119/153 (78%)	106 (89%)	12 (10%)	1 (1%)	19 53
2	D	126/134 (94%)	105 (83%)	18 (14%)	3 (2%)	6 26
3	E	110/114 (96%)	87 (79%)	22 (20%)	1 (1%)	17 51
4	G	410/489 (84%)	351 (86%)	50 (12%)	9 (2%)	6 28
5	H	223/244 (91%)	200 (90%)	20 (9%)	3 (1%)	12 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	L	209/217 (96%)	184 (88%)	22 (10%)	3 (1%)	11 39
All	All	1197/1351 (89%)	1033 (86%)	144 (12%)	20 (2%)	9 34

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	65	VAL
4	G	70	ALA
4	G	354	PRO
6	L	101	ALA
4	G	235	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	107/130 (82%)	104 (97%)	3 (3%)	43 74
2	D	107/112 (96%)	103 (96%)	4 (4%)	34 66
3	E	98/100 (98%)	94 (96%)	4 (4%)	30 64
4	G	375/433 (87%)	361 (96%)	14 (4%)	34 66
5	H	197/212 (93%)	188 (95%)	9 (5%)	27 60
6	L	175/181 (97%)	171 (98%)	4 (2%)	50 78
All	All	1059/1168 (91%)	1021 (96%)	38 (4%)	35 67

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	293	GLU
4	G	448	ASN
6	L	49	TYR
4	G	416	LEU
4	G	456	ARG

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

Mol	Chain	Res	Type
4	G	103	GLN
4	G	374	HIS
4	G	463	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

20 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	$\#\|Z\| > 2$
7	NAG	A	1	4,7	14,14,15	0.47	0	17,19,21	0.44	0
7	NAG	A	2	7	14,14,15	0.48	0	17,19,21	1.20	1 (5%)
7	BMA	A	3	7	11,11,12	0.55	0	15,15,17	0.69	0
7	MAN	A	4	7	11,11,12	0.88	0	15,15,17	1.03	2 (13%)
7	MAN	A	5	7	11,11,12	1.47	1 (9%)	15,15,17	1.71	3 (20%)
7	MAN	A	6	7	11,11,12	0.66	0	15,15,17	0.98	2 (13%)
8	NAG	C	1	8,4	14,14,15	0.29	0	17,19,21	0.41	0
8	NAG	C	2	8	14,14,15	0.24	0	17,19,21	0.43	0
8	NAG	F	1	8,4	14,14,15	0.33	0	17,19,21	0.57	0
8	NAG	F	2	8	14,14,15	0.26	0	17,19,21	0.43	0
9	NAG	I	1	9,4	14,14,15	0.55	0	17,19,21	1.37	2 (11%)
9	MAN	I	10	9	11,11,12	1.05	0	15,15,17	1.23	2 (13%)
9	NAG	I	2	9	14,14,15	0.22	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BMA	I	3	9	11,11,12	0.95	1 (9%)	15,15,17	0.89	0
9	MAN	I	4	9	11,11,12	0.67	0	15,15,17	1.23	2 (13%)
9	MAN	I	5	9	11,11,12	0.66	0	15,15,17	0.98	2 (13%)
9	MAN	I	6	9	11,11,12	0.76	0	15,15,17	0.88	1 (6%)
9	MAN	I	7	9	11,11,12	0.70	0	15,15,17	0.90	1 (6%)
9	MAN	I	8	9	11,11,12	0.88	1 (9%)	15,15,17	1.00	1 (6%)
9	MAN	I	9	9	11,11,12	0.78	0	15,15,17	1.09	2 (13%)

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
7	NAG	A	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	5/6/23/26	0/1/1/1
7	BMA	A	3	7	-	2/2/19/22	0/1/1/1
7	MAN	A	4	7	-	2/2/19/22	0/1/1/1
7	MAN	A	5	7	-	1/2/19/22	0/1/1/1
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1
8	NAG	C	1	8,4	-	0/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
8	NAG	F	1	8,4	-	0/6/23/26	0/1/1/1
8	NAG	F	2	8	-	2/6/23/26	0/1/1/1
9	NAG	I	1	9,4	-	3/6/23/26	0/1/1/1
9	MAN	I	10	9	-	0/2/19/22	0/1/1/1
9	NAG	I	2	9	-	2/6/23/26	0/1/1/1
9	BMA	I	3	9	-	0/2/19/22	0/1/1/1
9	MAN	I	4	9	-	2/2/19/22	0/1/1/1
9	MAN	I	5	9	-	1/2/19/22	0/1/1/1
9	MAN	I	6	9	-	0/2/19/22	0/1/1/1
9	MAN	I	7	9	-	0/2/19/22	0/1/1/1
9	MAN	I	8	9	-	2/2/19/22	0/1/1/1
9	MAN	I	9	9	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	5	MAN	C1-C2	4.12	1.61	1.52
9	I	3	BMA	O5-C1	-2.32	1.40	1.43
9	I	8	MAN	C1-C2	2.26	1.57	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	1	NAG	C2-N2-C7	4.19	128.87	122.90
7	A	5	MAN	C1-O5-C5	4.11	117.76	112.19
7	A	2	NAG	C2-N2-C7	4.11	128.75	122.90
7	A	5	MAN	C1-C2-C3	3.85	114.40	109.67
9	I	4	MAN	C1-O5-C5	3.23	116.56	112.19

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	2	NAG	O5-C5-C6-O6
9	I	2	NAG	O5-C5-C6-O6
9	I	4	MAN	O5-C5-C6-O6
7	A	3	BMA	O5-C5-C6-O6
9	I	9	MAN	C4-C5-C6-O6

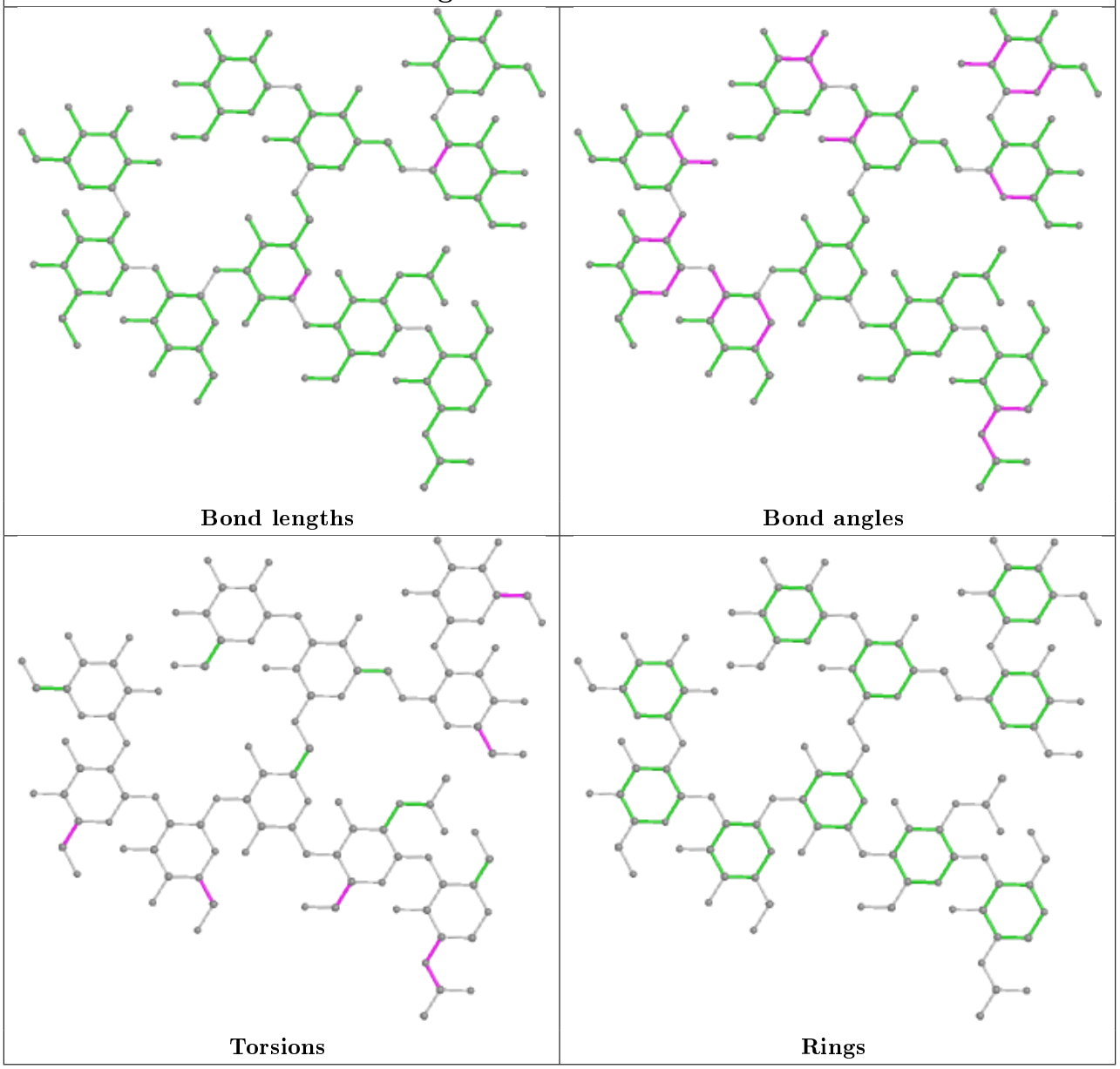
There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1	NAG	2	0
8	F	1	NAG	1	0
7	A	5	MAN	1	0
7	A	4	MAN	1	0
7	A	2	NAG	2	0
9	I	1	NAG	2	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 I



5.6 Ligand geometry (i)

15 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	$\#\|Z\|>2$
10	NAG	G	617	4	14,14,15	0.30	0	17,19,21	0.46	0
10	NAG	B	701	1	14,14,15	0.36	0	17,19,21	0.51	0
10	NAG	G	632	4	14,14,15	0.83	1 (7%)	17,19,21	1.58	1 (5%)
10	NAG	G	616	4	14,14,15	0.27	0	17,19,21	0.51	0
11	JYS	G	633	-	30,32,32	5.65	16 (53%)	38,46,46	1.81	7 (18%)
10	NAG	G	629	4	14,14,15	0.33	0	17,19,21	0.57	0
10	NAG	G	610	4	14,14,15	0.25	0	17,19,21	0.39	0
10	NAG	G	611	4	14,14,15	0.32	0	17,19,21	0.53	0
10	NAG	G	628	4	14,14,15	0.30	0	17,19,21	0.46	0
10	NAG	G	630	4	14,14,15	0.19	0	17,19,21	0.38	0
10	NAG	G	609	4	14,14,15	0.26	0	17,19,21	0.47	0
10	NAG	B	702	1	14,14,15	0.32	0	17,19,21	0.47	0
10	NAG	G	612	4	14,14,15	0.24	0	17,19,21	0.44	0
10	NAG	G	615	4	14,14,15	0.31	0	17,19,21	0.50	0
10	NAG	G	631	4	14,14,15	0.33	0	17,19,21	0.58	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
10	NAG	G	617	4	-	1/6/23/26	0/1/1/1
10	NAG	B	701	1	-	0/6/23/26	0/1/1/1
10	NAG	G	632	4	-	3/6/23/26	0/1/1/1
10	NAG	G	616	4	-	2/6/23/26	0/1/1/1
11	JYS	G	633	-	-	4/16/30/30	0/4/4/4
10	NAG	G	629	4	-	1/6/23/26	0/1/1/1
10	NAG	G	610	4	-	2/6/23/26	0/1/1/1
10	NAG	G	611	4	-	0/6/23/26	0/1/1/1
10	NAG	G	628	4	-	2/6/23/26	0/1/1/1
10	NAG	G	630	4	-	4/6/23/26	0/1/1/1
10	NAG	G	609	4	-	1/6/23/26	0/1/1/1
10	NAG	B	702	1	-	1/6/23/26	0/1/1/1
10	NAG	G	612	4	-	2/6/23/26	0/1/1/1
10	NAG	G	615	4	-	1/6/23/26	0/1/1/1
10	NAG	G	631	4	-	2/6/23/26	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	633	JYS	C02-C03	17.00	1.57	1.41
11	G	633	JYS	C01-C02	11.92	1.50	1.36
11	G	633	JYS	C05-C04	8.16	1.59	1.43
11	G	633	JYS	C21-C16	8.16	1.53	1.39
11	G	633	JYS	C17-C16	7.97	1.52	1.39

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	G	632	NAG	C1-O5-C5	6.08	120.42	112.19
11	G	633	JYS	F22-C02-C03	4.95	119.40	117.40
11	G	633	JYS	C01-C02-C03	-4.64	120.72	123.09
11	G	633	JYS	C09-C10-N24	4.62	123.07	118.52
11	G	633	JYS	C11-C12-N25	3.57	118.09	110.44

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	G	633	JYS	C08-C09-C10-O27
11	G	633	JYS	O26-C09-C10-N24
11	G	633	JYS	O26-C09-C10-O27
10	G	631	NAG	C4-C5-C6-O6
10	G	612	NAG	O5-C5-C6-O6

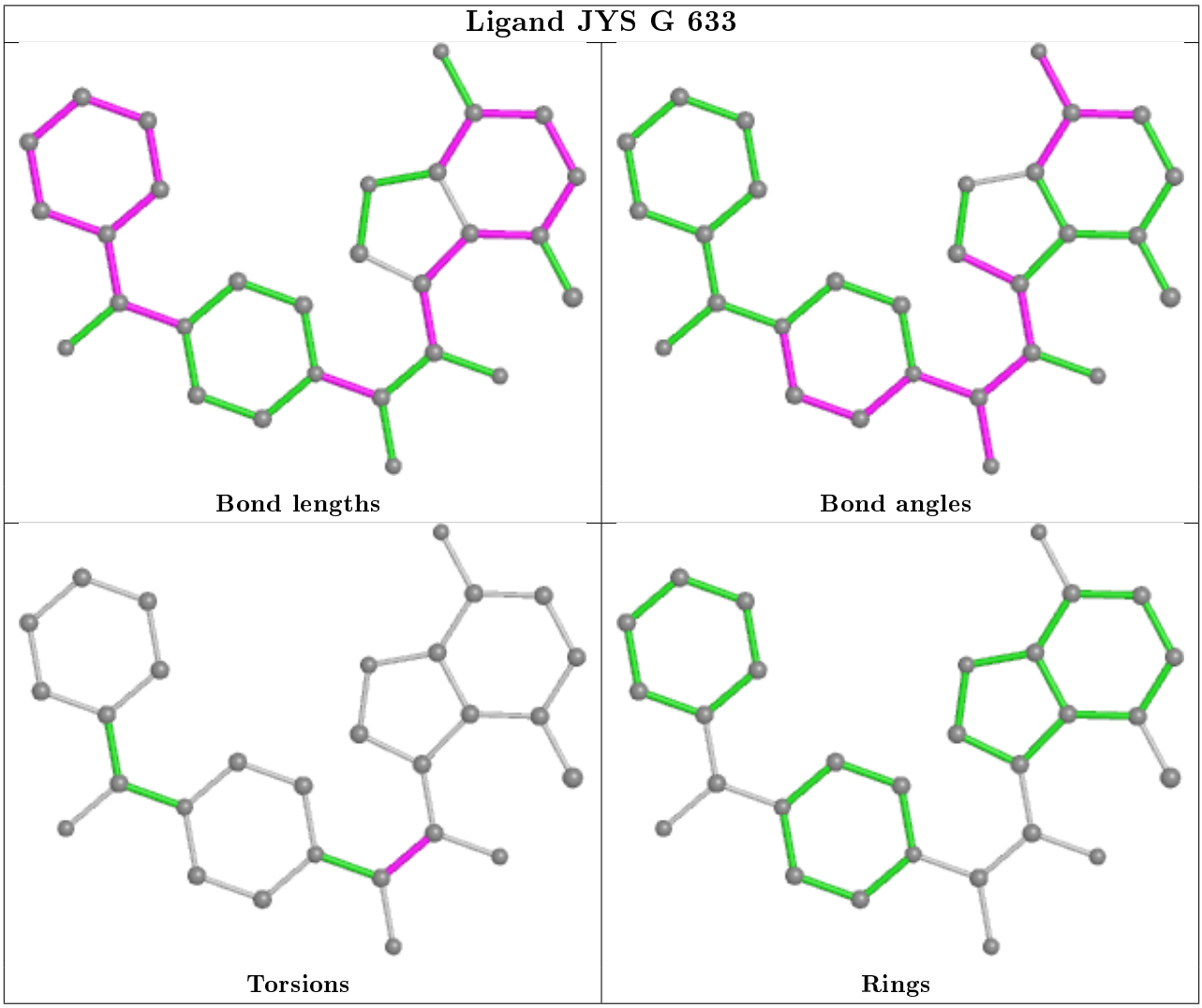
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	G	633	JYS	2	0
10	G	611	NAG	1	0
10	G	630	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.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	B	123/153 (80%)	-0.38	1 (0%)	86	73	9, 29, 83, 109	0
2	D	128/134 (95%)	-0.34	2 (1%)	72	55	24, 66, 112, 122	0
3	E	112/114 (98%)	-0.42	3 (2%)	54	38	21, 60, 105, 125	0
4	G	424/489 (86%)	-0.48	0	100	100	9, 41, 85, 123	0
5	H	227/244 (93%)	-0.56	0	100	100	19, 51, 89, 108	0
6	L	211/217 (97%)	-0.61	0	100	100	14, 39, 61, 97	0
All	All	1225/1351 (90%)	-0.49	6 (0%)	91	81	9, 45, 96, 125	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	541	ALA	3.0
3	E	107	GLY	2.8
3	E	106(A)	LEU	2.8
2	D	41	ALA	2.1
2	D	8	GLY	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

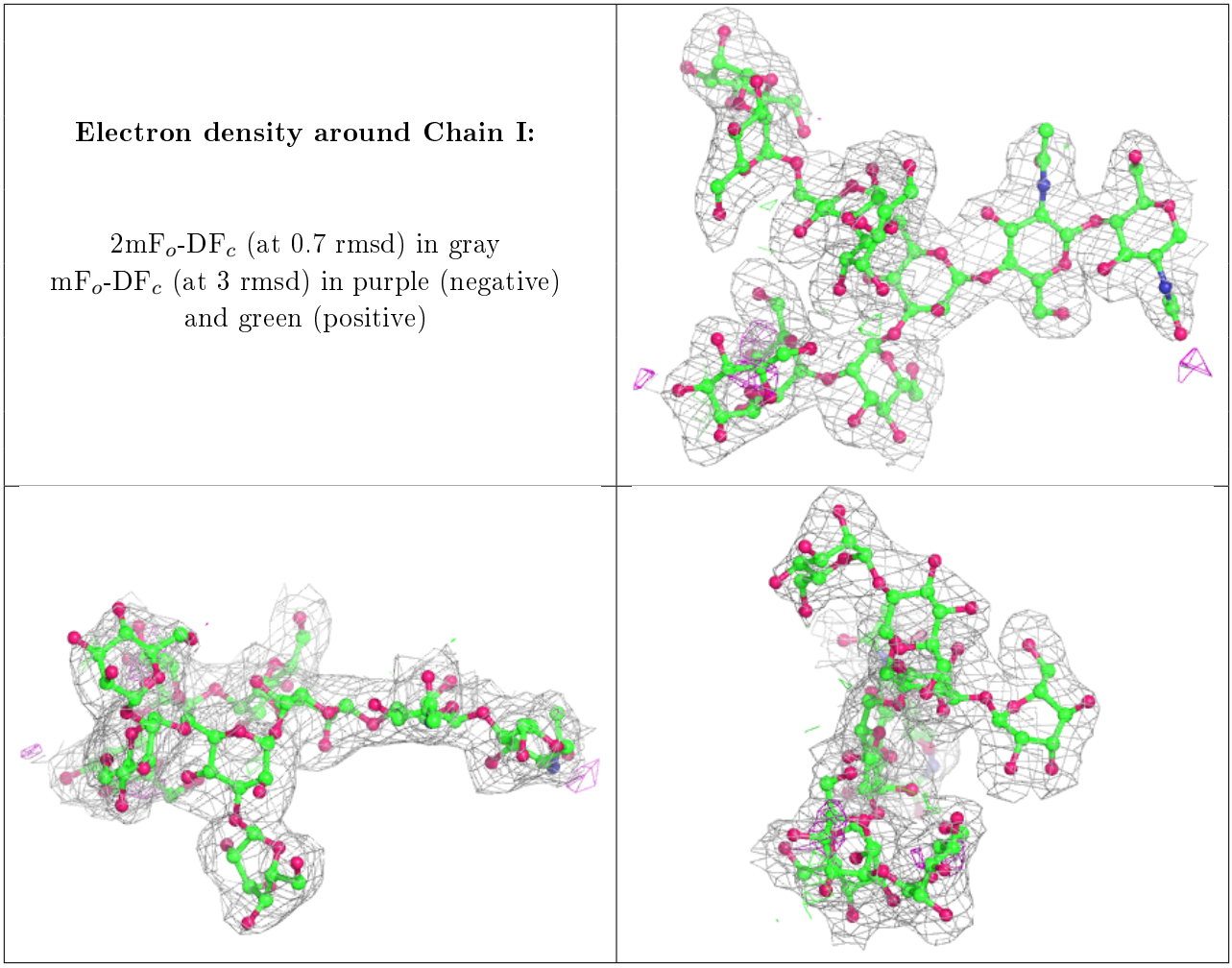
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
7	MAN	A	4	11/12	0.91	0.12	68,80,101,113	0
7	MAN	A	5	11/12	0.93	0.14	57,88,112,117	0
8	NAG	F	2	14/15	0.95	0.14	37,49,61,78	0
9	MAN	I	6	11/12	0.95	0.20	44,68,95,98	0
8	NAG	C	2	14/15	0.95	0.15	50,67,92,94	0
9	MAN	I	9	11/12	0.95	0.22	69,90,103,126	0
9	MAN	I	8	11/12	0.95	0.15	62,82,103,111	0
8	NAG	C	1	14/15	0.96	0.11	27,56,65,66	0
9	MAN	I	5	11/12	0.97	0.14	22,46,53,61	0
9	NAG	I	2	14/15	0.97	0.15	34,67,78,81	0
9	MAN	I	7	11/12	0.97	0.10	39,62,105,109	0
9	MAN	I	10	11/12	0.97	0.10	47,80,99,101	0
9	NAG	I	1	14/15	0.98	0.14	53,70,105,123	0
7	NAG	A	2	14/15	0.98	0.13	27,46,68,78	0
9	BMA	I	3	11/12	0.98	0.09	52,63,71,72	0
7	MAN	A	6	11/12	0.98	0.12	28,46,51,65	0
7	BMA	A	3	11/12	0.98	0.13	18,55,69,71	0
8	NAG	F	1	14/15	0.98	0.12	14,47,60,72	0
7	NAG	A	1	14/15	0.99	0.14	19,30,41,44	0
9	MAN	I	4	11/12	0.99	0.12	31,39,52,60	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 I:

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



6.4 Ligands

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
10	NAG	B	701	14/15	0.86	0.29	78,107,137,145	0
10	NAG	G	630	14/15	0.88	0.33	74,114,142,151	0
10	NAG	G	610	14/15	0.89	0.31	101,125,132,134	0
10	NAG	B	702	14/15	0.91	0.19	75,108,130,131	0
10	NAG	G	609	14/15	0.95	0.12	43,69,96,99	0
10	NAG	G	632	14/15	0.95	0.17	51,70,97,115	0
10	NAG	G	612	14/15	0.95	0.17	39,85,113,119	0
10	NAG	G	615	14/15	0.95	0.17	42,95,107,109	0
10	NAG	G	631	14/15	0.95	0.15	50,78,97,100	0
10	NAG	G	616	14/15	0.96	0.15	25,45,58,64	0

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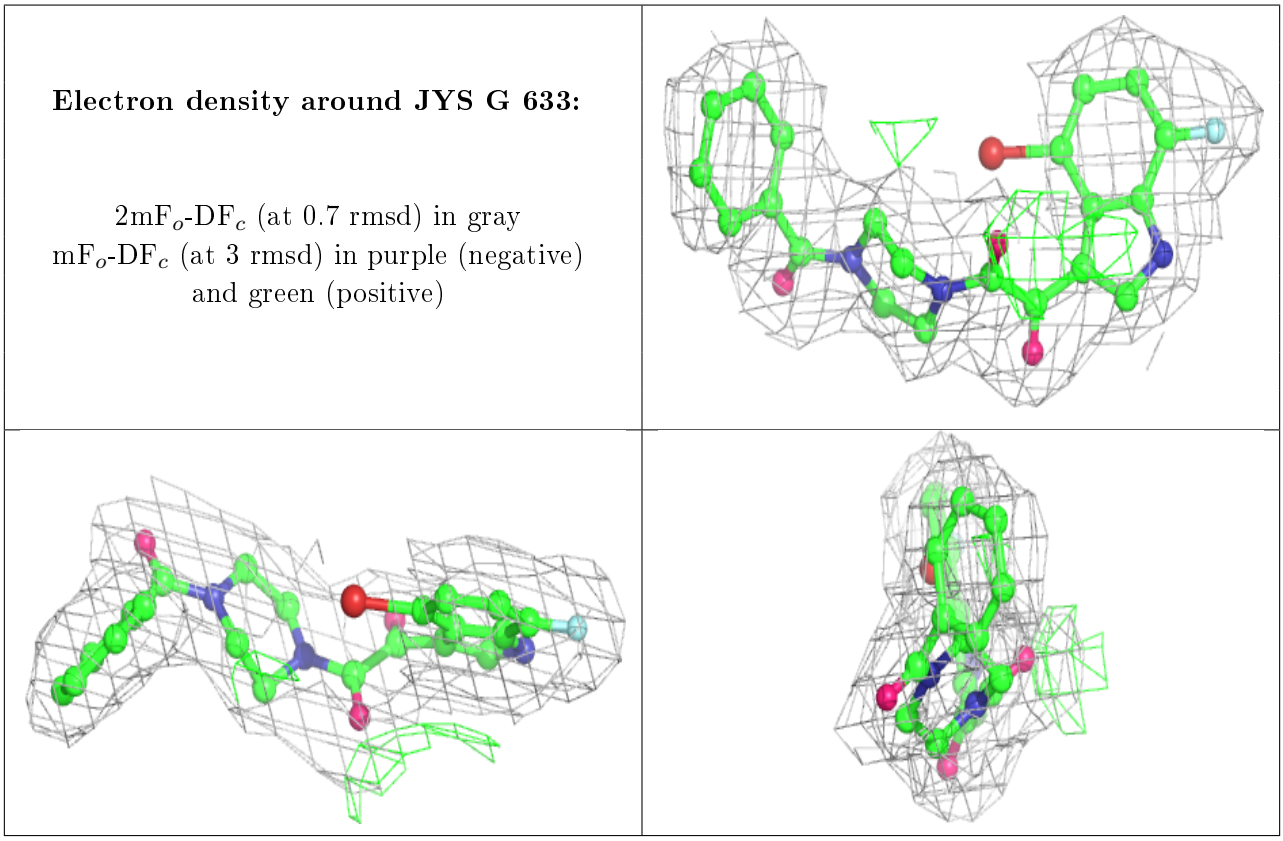
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	NAG	G	628	14/15	0.96	0.18	55,93,119,120	0
10	NAG	G	629	14/15	0.97	0.15	27,43,63,65	0
10	NAG	G	617	14/15	0.97	0.12	22,46,64,66	0
10	NAG	G	611	14/15	0.97	0.15	51,62,85,95	0
11	JYS	G	633	29/29	0.98	0.13	14,47,69,74	0

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 JYS G 633:

$2mF_o$-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

There are no such residues in this entry.