Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 11:49 PM BST

PDB ID	:	6MU7
Title	:	Crystal Structure of HIV-1 BG505 SOSIP.664 Prefusion Env Trimer Bound to Small Molecule HIV-1 Entry Inhibitor BMS-818251 in Complex with Human Antibodies 3H109L and 35O22 at 3.1 Angstrom
Authors	:	Lai, Y.-T.; Kwong, P.D.
Deposited on	:	2018-10-22
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

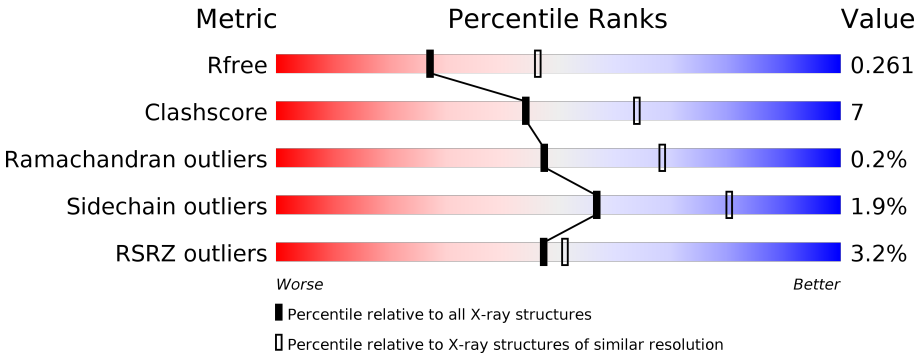
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	3% 76% 10% 13%
2	D	134	8% 73% 22% •
3	E	114	4% 85% 7% 8%
4	G	481	3% 74% 17% • 8%
5	H	244	2% 73% 18% • 7%
6	L	217	78% 18% •

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Mol	Chain	Length	Quality of chain
7	A	6	17% 50% 33%
8	C	3	67% 33%
8	F	3	100%
9	I	2	100%
9	J	2	100%
9	M	2	50% 50%
10	K	10	10% 60% 30%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	JYY	G	637	X	-	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 10225 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	133	Total	C	N	O	S	0	0	0
			1056	673	182	195	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- 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	105	Total	C	N	O	S	0	0	0
			805	506	133	160	6			

- Molecule 4 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	442	Total	C	N	O	S	0	0	0
			3479	2186	617	648	28			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	137	ALA	ASN	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

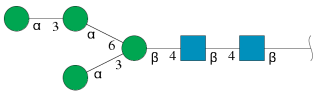
- Molecule 5 is a protein called 3H109L Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	226	Total	C	N	O	S	0	0	0
			1715	1093	278	338	6			

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

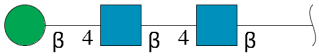
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	211	Total	C	N	O	S	0	0	0
			1604	1009	276	312	7			

- 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 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
8	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

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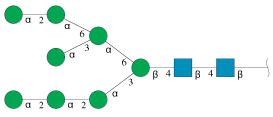
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

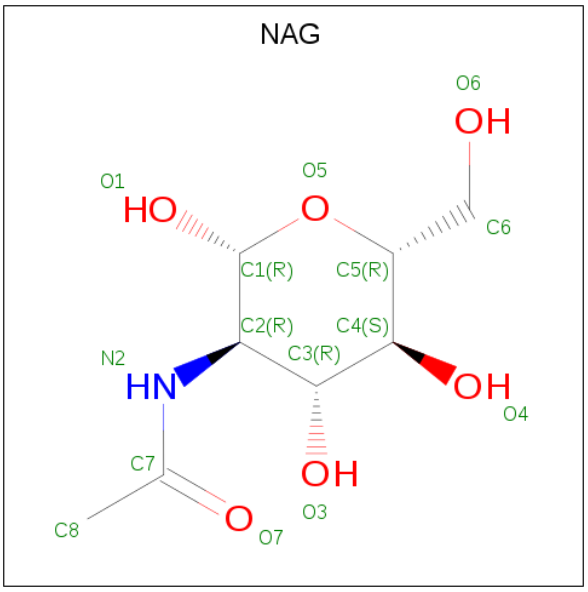
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 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.



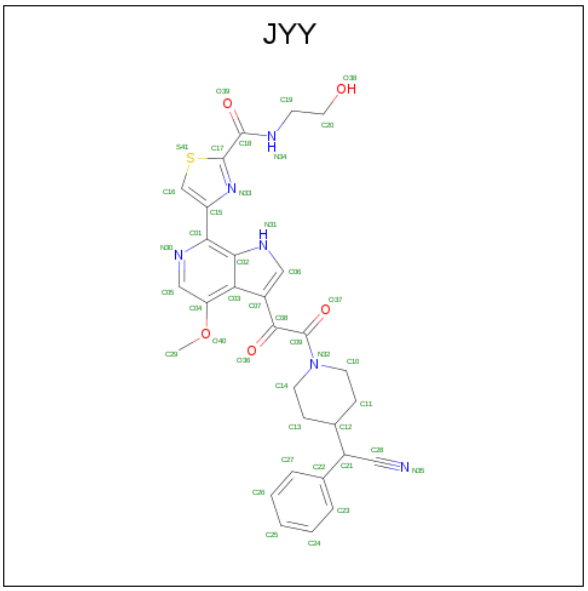
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 12 is 4-{3-[{4-[(R)-cyano(phenyl)methyl]piperidin-1-yl}(oxo)acetyl]-4-methoxy-1 H-pyrrolo[2,3-c]pyridin-7-yl}-N-(2-hydroxyethyl)-1,3-thiazole-2-carboxamide (three-letter code: JYY) (formula: $C_{29}H_{28}N_6O_5S$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	G	1	Total	C	N	O	S	0	0
			41	29	6	5	1		

- Molecule 13 is water.

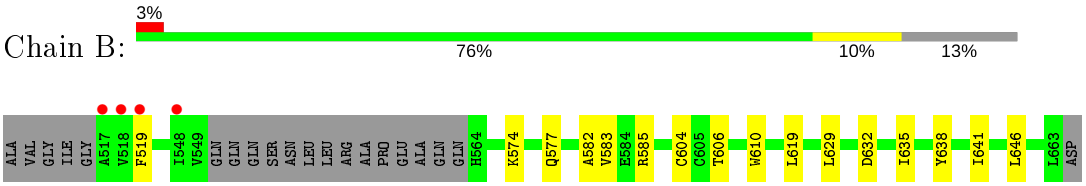
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	3	Total	O	0	0
			3	3		
13	D	3	Total	O	0	0
			3	3		
13	E	1	Total	O	0	0
			1	1		
13	G	5	Total	O	0	0
			5	5		
13	L	1	Total	O	0	0
			1	1		

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.

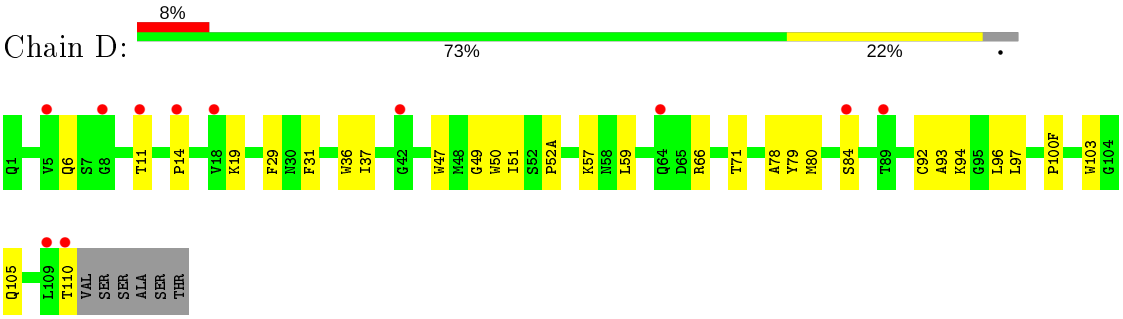
- Molecule 1: Envelope glycoprotein gp160

Chain B:



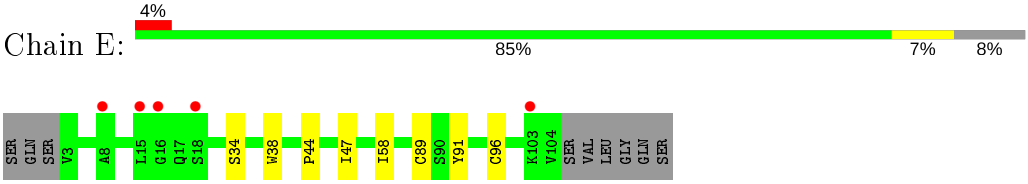
- Molecule 2: 35O22 scFv heavy chain portion

Chain D:



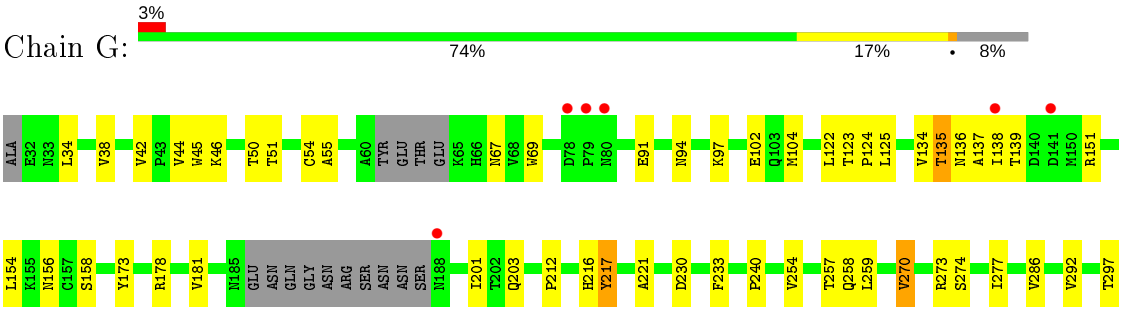
- Molecule 3: 35O22 scFv light chain portion

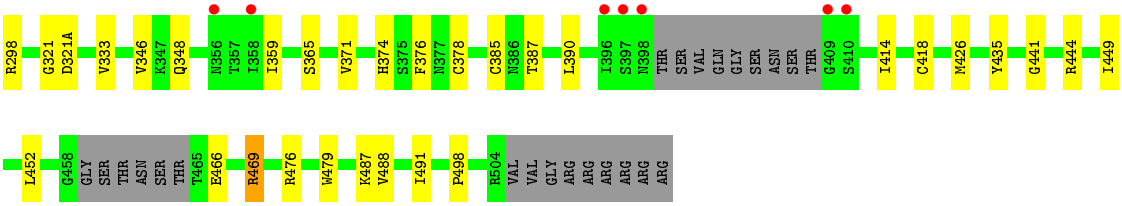
Chain E:



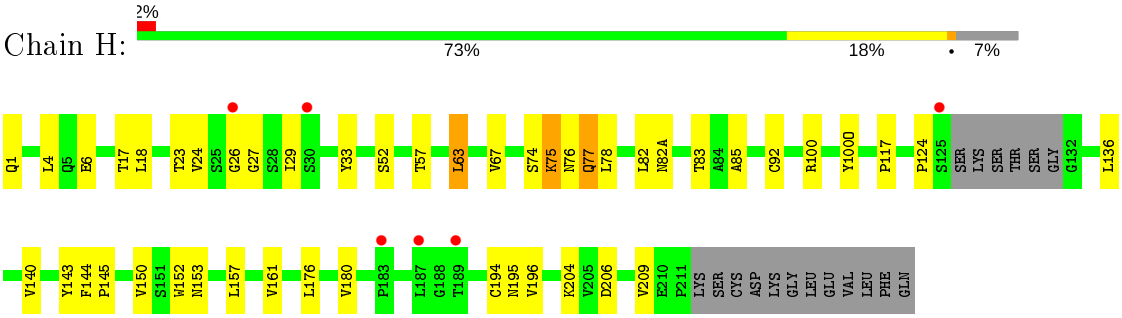
- Molecule 4: Envelope glycoprotein gp160

Chain G:

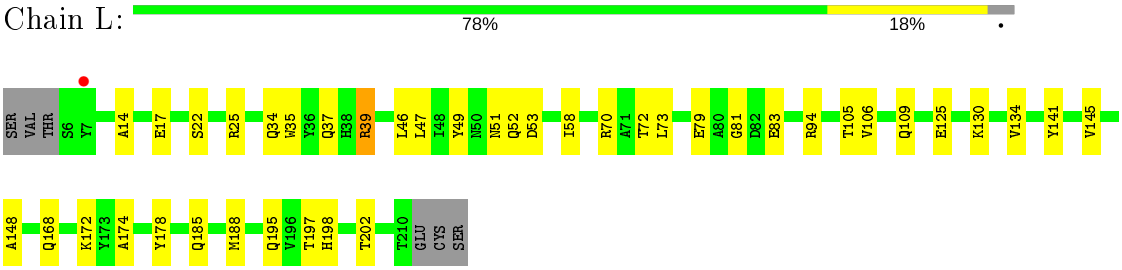




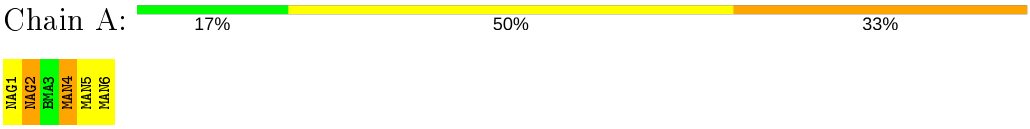
• Molecule 5: 3H109L Fab heavy chain



• Molecule 6: 3H109L Fab light chain



• 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

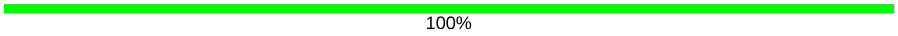


• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

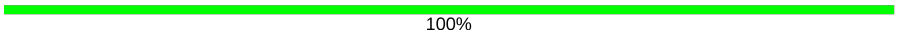
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

• Molecule 10: 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 K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	131.51Å 131.51Å 314.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.05 – 2.50 43.05 – 2.46	Depositor EDS
% Data completeness (in resolution range)	38.4 (43.05-2.50) 36.4 (43.05-2.46)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.223 , 0.261 0.223 , 0.261	Depositor DCC
R_{free} test set	2027 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 23.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	10225	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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, JYY, NAG, 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	0.23	0/1075	0.38	0/1458
2	D	0.24	0/1021	0.46	0/1390
3	E	0.25	0/829	0.46	0/1133
4	G	0.25	0/3550	0.45	0/4815
5	H	0.25	0/1758	0.46	0/2397
6	L	0.25	0/1647	0.45	0/2247
All	All	0.25	0/9880	0.45	0/13440

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	1056	0	1049	11	0
2	D	994	0	952	18	0
3	E	805	0	752	3	0
4	G	3479	0	3423	57	0
5	H	1715	0	1685	27	0
6	L	1604	0	1553	26	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	39	0	34	1	0
8	F	39	0	34	0	0
9	I	28	0	25	0	0
9	J	28	0	25	0	0
9	M	28	0	25	0	0
10	K	116	0	97	3	0
11	B	42	0	39	0	0
11	D	14	0	13	0	0
11	G	112	0	104	1	0
12	G	41	0	0	1	0
13	B	3	0	0	0	0
13	D	3	0	0	1	0
13	E	1	0	0	0	0
13	G	5	0	0	0	0
13	L	1	0	0	0	0
All	All	10225	0	9871	133	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 7.

All (133) 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:274:SER:HB3	4:G:277:ILE:HG12	1.65	0.79
2:D:6:GLN:H	2:D:105:GLN:HE22	1.38	0.71
4:G:137:ALA:H	4:G:151:ARG:HH21	1.38	0.70
4:G:257:THR:HG22	4:G:258:GLN:HG3	1.79	0.65
5:H:136:LEU:HD13	5:H:209:VAL:HG21	1.79	0.65
6:L:34:GLN:HG3	6:L:49:TYR:HA	1.79	0.64
4:G:122:LEU:HD11	4:G:203:GLN:HB3	1.81	0.63
5:H:100(O):TYR:HB3	6:L:34:GLN:HE21	1.64	0.61
4:G:365:SER:HB3	4:G:469:ARG:HE	1.64	0.61
4:G:292:VAL:HG13	4:G:449:ILE:HB	1.82	0.61
1:B:585:ARG:NH2	4:G:491:ILE:O	2.33	0.61
4:G:178:ARG:NH1	4:G:181:VAL:O	2.34	0.60
6:L:148:ALA:HB3	6:L:195:GLN:HB2	1.84	0.60
5:H:161:VAL:HA	5:H:180:VAL:HG12	1.84	0.60
7:A:2:NAG:H3	7:A:2:NAG:H83	1.86	0.58
4:G:233:PHE:O	4:G:273:ARG:NH1	2.33	0.58
4:G:277:ILE:HG13	11:G:613:NAG:H81	1.85	0.58
4:G:122:LEU:HB2	4:G:201:ILE:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:63:LEU:HD13	5:H:67:VAL:HG21	1.87	0.57
6:L:52:GLN:NE2	6:L:53:ASP:OD1	2.38	0.56
6:L:22:SER:HA	6:L:72:THR:HG22	1.88	0.56
4:G:359:ILE:HG22	4:G:466:GLU:HB2	1.87	0.55
4:G:201:ILE:HD11	4:G:435:TYR:HB2	1.88	0.55
4:G:138:ILE:HG23	4:G:139:THR:H	1.71	0.54
6:L:83:GLU:HG3	6:L:106:VAL:HG23	1.88	0.54
1:B:632:ASP:HA	1:B:635:ILE:HG22	1.89	0.54
4:G:476:ARG:HA	4:G:479:TRP:CD1	2.43	0.54
5:H:74:SER:OG	5:H:75:LYS:NZ	2.40	0.54
4:G:298:ARG:NH2	4:G:441:GLY:O	2.41	0.54
5:H:17:THR:HA	5:H:82(A):ASN:HA	1.89	0.53
4:G:270:VAL:HG13	4:G:348:GLN:HG3	1.90	0.53
4:G:333:VAL:HG11	4:G:390:LEU:HD21	1.90	0.53
5:H:100:ARG:NH2	10:K:4:MAN:O6	2.42	0.53
4:G:257:THR:HG21	4:G:371:VAL:HA	1.90	0.53
5:H:117:PRO:HB3	5:H:143:TYR:HB3	1.91	0.53
5:H:4:LEU:HD23	5:H:92:CYS:SG	2.48	0.52
1:B:629:LEU:HD23	4:G:44:VAL:HG23	1.89	0.52
5:H:24:VAL:HB	5:H:76:ASN:HB3	1.91	0.52
6:L:39:ARG:NH1	6:L:81:GLY:O	2.42	0.52
5:H:195:ASN:ND2	5:H:206:ASP:OD2	2.41	0.52
2:D:51:ILE:HG13	2:D:57:LYS:HB3	1.91	0.52
2:D:36:TRP:CZ3	2:D:92:CYS:HB3	2.44	0.52
4:G:50:THR:HG22	4:G:488:VAL:HG11	1.92	0.51
6:L:109:GLN:HB2	6:L:141:TYR:CE1	2.46	0.51
5:H:29:ILE:HD11	5:H:78:LEU:HB3	1.93	0.50
6:L:14:ALA:HB3	6:L:17:GLU:HG3	1.92	0.50
3:E:38:TRP:CE2	3:E:44:PRO:HG3	2.47	0.50
6:L:47:LEU:HA	6:L:58:ILE:HD13	1.92	0.49
4:G:102:GLU:OE2	4:G:476:ARG:NH1	2.45	0.49
4:G:67:ASN:HD22	4:G:69:TRP:HD1	1.59	0.49
4:G:333:VAL:HG13	4:G:414:ILE:HG13	1.94	0.49
5:H:150:VAL:HG22	5:H:196:VAL:HG22	1.94	0.49
5:H:153:ASN:HB2	5:H:157:LEU:H	1.76	0.49
3:E:47:ILE:HD13	3:E:58:ILE:HD12	1.94	0.49
4:G:135:THR:HG21	6:L:94:ARG:HE	1.77	0.48
2:D:96:LEU:HG	2:D:97:LEU:HG	1.95	0.48
6:L:83:GLU:HG2	6:L:105:THR:HA	1.95	0.48
5:H:23:THR:HG22	5:H:77:GLN:HG2	1.94	0.48
4:G:91:GLU:OE1	4:G:487:LYS:NZ	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:104:MET:HB2	4:G:217:TYR:HE2	1.78	0.48
1:B:610:TRP:CD2	4:G:498:PRO:HB3	2.49	0.47
4:G:158:SER:HA	4:G:173:TYR:HA	1.95	0.47
1:B:606:THR:HG21	1:B:646:LEU:HD22	1.96	0.47
4:G:212:PRO:HG3	4:G:254:VAL:HG22	1.96	0.47
2:D:50:TRP:CH2	7:A:4:MAN:H62	2.49	0.47
4:G:55:ALA:HB3	4:G:216:HIS:HB2	1.97	0.47
2:D:29:PHE:CE2	2:D:52(A):PRO:HB3	2.49	0.47
1:B:577:GLN:HG2	4:G:51:THR:HG21	1.97	0.46
5:H:124:PRO:HD3	5:H:136:LEU:HB3	1.98	0.46
5:H:27:GLY:O	5:H:76:ASN:ND2	2.48	0.46
4:G:138:ILE:HG22	4:G:151:ARG:HG2	1.97	0.46
4:G:346:VAL:HG22	4:G:359:ILE:HD11	1.96	0.46
2:D:11:THR:HB	2:D:110:THR:HA	1.97	0.46
2:D:50:TRP:HH2	7:A:4:MAN:H62	1.81	0.46
5:H:140:VAL:O	5:H:176:LEU:N	2.40	0.46
4:G:230:ASP:HB3	4:G:233:PHE:HB2	1.97	0.46
6:L:197:THR:HA	6:L:202:THR:HA	1.98	0.46
4:G:123:THR:N	4:G:124:PRO:HD2	2.31	0.45
5:H:152:TRP:HB3	5:H:157:LEU:HD23	1.99	0.45
4:G:286:VAL:HG22	4:G:452:LEU:HB2	1.98	0.45
2:D:19:LYS:HD2	2:D:79:TYR:HB3	1.97	0.45
5:H:1:GLN:O	5:H:26:GLY:HA3	2.16	0.45
6:L:145:VAL:HG12	6:L:198:HIS:HB2	1.98	0.45
4:G:376:PHE:HE2	4:G:378:CYS:HB2	1.82	0.45
6:L:70:ARG:HG3	6:L:72:THR:HG23	1.99	0.45
6:L:37:GLN:HB2	6:L:47:LEU:HD11	1.98	0.45
4:G:297:THR:HB	4:G:444:ARG:HG3	1.98	0.45
6:L:168:GLN:N	6:L:172:LYS:O	2.38	0.45
4:G:45:TRP:O	4:G:46:LYS:HD2	2.16	0.44
4:G:94:ASN:HB3	4:G:97:LYS:HG2	1.98	0.44
5:H:6:GLU:OE1	5:H:6:GLU:N	2.50	0.44
2:D:19:LYS:HA	2:D:80:MET:O	2.18	0.44
1:B:604:CYS:SG	4:G:38:VAL:HB	2.57	0.44
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.52	0.44
6:L:134:VAL:HG12	6:L:178:TYR:CD2	2.53	0.44
5:H:18:LEU:N	5:H:82:LEU:O	2.49	0.44
4:G:135:THR:HG21	6:L:94:ARG:HB3	1.99	0.44
6:L:46:LEU:HD21	6:L:49:TYR:HB3	2.00	0.43
1:B:619:LEU:HD11	4:G:34:LEU:HD21	2.00	0.43
4:G:134:VAL:HB	4:G:156:ASN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:75:LYS:HB2	5:H:76:ASN:H	1.67	0.43
5:H:18:LEU:HD22	5:H:82:LEU:HB3	2.00	0.43
6:L:185:GLN:HA	6:L:188:MET:HG2	2.01	0.43
4:G:122:LEU:HB3	4:G:125:LEU:HD12	2.01	0.43
10:K:1:NAG:H3	10:K:1:NAG:H83	2.01	0.43
6:L:168:GLN:OE1	6:L:174:ALA:HB2	2.19	0.43
1:B:610:TRP:CG	4:G:498:PRO:HB3	2.54	0.43
1:B:582:ALA:HB1	4:G:221:ALA:HB3	2.01	0.43
2:D:37:ILE:HG13	2:D:103:TRP:CH2	2.54	0.43
6:L:51:ASN:ND2	10:K:5:MAN:O4	2.48	0.42
1:B:638:TYR:HA	1:B:641:ILE:HD13	2.01	0.42
5:H:144:PHE:HA	5:H:145:PRO:HA	1.78	0.42
2:D:94:LYS:NZ	13:D:301:HOH:O	2.52	0.42
4:G:42:VAL:HG23	4:G:44:VAL:HG12	2.01	0.42
5:H:83:THR:HG23	5:H:85:ALA:H	1.84	0.42
2:D:14:PRO:HG3	2:D:84:SER:HB3	2.01	0.42
4:G:376:PHE:CE2	4:G:378:CYS:HB2	2.55	0.42
4:G:136:ASN:OD1	4:G:151:ARG:HD2	2.20	0.42
5:H:33:TYR:CD2	5:H:52:SER:HA	2.55	0.42
4:G:122:LEU:HD13	4:G:125:LEU:HD12	2.01	0.41
4:G:385:CYS:HA	4:G:418:CYS:HA	2.02	0.41
4:G:321(A):ASP:HB2	8:C:1:NAG:H83	2.00	0.41
2:D:93:ALA:HB3	2:D:100(F):PRO:HB3	2.02	0.41
2:D:6:GLN:H	2:D:105:GLN:NE2	2.13	0.41
2:D:71:THR:HG22	2:D:78:ALA:HA	2.02	0.41
3:E:34:SER:HB3	3:E:91:TYR:HE1	1.84	0.41
6:L:125:GLU:HG2	6:L:130:LYS:O	2.20	0.41
4:G:387:THR:HG22	4:G:390:LEU:HD12	2.03	0.40
4:G:426:MET:HG3	12:G:637:JYY:O37	2.21	0.40
6:L:35:TRP:CD2	6:L:73:LEU:HB2	2.56	0.40
2:D:31:PHE:HA	7:A:1:NAG:H62	2.03	0.40
6:L:79:GLU:O	6:L:106:VAL:HG21	2.21	0.40
4:G:259:LEU:HB2	4:G:374:HIS:CE1	2.56	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	B	129/153 (84%)	120 (93%)	9 (7%)	0	100 100
2	D	126/134 (94%)	110 (87%)	16 (13%)	0	100 100
3	E	103/114 (90%)	88 (85%)	15 (15%)	0	100 100
4	G	432/481 (90%)	400 (93%)	29 (7%)	3 (1%)	22 39
5	H	222/244 (91%)	208 (94%)	14 (6%)	0	100 100
6	L	209/217 (96%)	195 (93%)	14 (7%)	0	100 100
All	All	1221/1343 (91%)	1121 (92%)	97 (8%)	3 (0%)	47 68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	135	THR
4	G	240	PRO
4	G	321	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	114/129 (88%)	111 (97%)	3 (3%)	46 72
2	D	107/112 (96%)	105 (98%)	2 (2%)	57 80
3	E	92/100 (92%)	90 (98%)	2 (2%)	52 77
4	G	393/427 (92%)	388 (99%)	5 (1%)	69 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	H	196/212 (92%)	190 (97%)	6 (3%)	40 67
6	L	175/181 (97%)	173 (99%)	2 (1%)	73 89
All	All	1077/1161 (93%)	1057 (98%)	20 (2%)	57 80

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	519	PHE
1	B	574	LYS
1	B	583	VAL
2	D	59	LEU
2	D	66	ARG
3	E	89	CYS
3	E	96	CYS
4	G	54	CYS
4	G	154	LEU
4	G	217	TYR
4	G	270	VAL
4	G	469	ARG
5	H	57	THR
5	H	63	LEU
5	H	75	LYS
5	H	77	GLN
5	H	194	CYS
5	H	204	LYS
6	L	25	ARG
6	L	39	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	$\#\|Z\|>2$
7	NAG	A	1	4,7	14,14,15	0.27	0	17,19,21	0.47	0
7	NAG	A	2	7	14,14,15	0.45	0	17,19,21	1.27	1 (5%)
7	BMA	A	3	7	11,11,12	0.77	0	15,15,17	0.75	0
7	MAN	A	4	7	11,11,12	1.37	2 (18%)	15,15,17	1.94	5 (33%)
7	MAN	A	5	7	11,11,12	1.61	2 (18%)	15,15,17	2.18	4 (26%)
7	MAN	A	6	7	11,11,12	0.64	0	15,15,17	1.00	2 (13%)
8	NAG	C	1	8,4	14,14,15	0.30	0	17,19,21	0.41	0
8	NAG	C	2	8	14,14,15	0.21	0	17,19,21	0.43	0
8	BMA	C	3	8	11,11,12	0.66	0	15,15,17	0.70	0
8	NAG	F	1	8,4	14,14,15	0.26	0	17,19,21	0.55	0
8	NAG	F	2	8	14,14,15	0.28	0	17,19,21	0.57	0
8	BMA	F	3	8	11,11,12	0.66	0	15,15,17	0.70	0
9	NAG	I	1	9,4	14,14,15	0.29	0	17,19,21	0.40	0
9	NAG	I	2	9	14,14,15	0.23	0	17,19,21	0.41	0
9	NAG	J	1	9,4	14,14,15	0.18	0	17,19,21	0.45	0
9	NAG	J	2	9	14,14,15	0.23	0	17,19,21	0.48	0
10	NAG	K	1	10,4	14,14,15	0.38	0	17,19,21	1.41	2 (11%)
10	MAN	K	10	10	11,11,12	1.08	0	15,15,17	1.13	1 (6%)
10	NAG	K	2	10	14,14,15	0.24	0	17,19,21	0.42	0
10	BMA	K	3	10	11,11,12	0.85	0	15,15,17	1.02	1 (6%)
10	MAN	K	4	10	11,11,12	0.73	1 (9%)	15,15,17	1.24	2 (13%)
10	MAN	K	5	10	11,11,12	0.61	0	15,15,17	0.95	2 (13%)
10	MAN	K	6	10	11,11,12	0.85	0	15,15,17	0.91	1 (6%)
10	MAN	K	7	10	11,11,12	0.79	0	15,15,17	0.96	1 (6%)
10	MAN	K	8	10	11,11,12	0.62	0	15,15,17	1.15	1 (6%)
10	MAN	K	9	10	11,11,12	0.87	1 (9%)	15,15,17	1.49	2 (13%)
9	NAG	M	1	9,4	14,14,15	0.38	0	17,19,21	0.67	1 (5%)
9	NAG	M	2	9	14,14,15	0.30	0	17,19,21	0.42	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
7	NAG	A	1	4,7	-	0/6/23/26	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	-	1/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
8	BMA	C	3	8	-	0/2/19/22	0/1/1/1
8	NAG	F	1	8,4	-	2/6/23/26	0/1/1/1
8	NAG	F	2	8	-	2/6/23/26	0/1/1/1
8	BMA	F	3	8	-	0/2/19/22	0/1/1/1
9	NAG	I	1	9,4	-	2/6/23/26	0/1/1/1
9	NAG	I	2	9	-	1/6/23/26	0/1/1/1
9	NAG	J	1	9,4	-	1/6/23/26	0/1/1/1
9	NAG	J	2	9	-	2/6/23/26	0/1/1/1
10	NAG	K	1	10,4	-	4/6/23/26	0/1/1/1
10	MAN	K	10	10	-	0/2/19/22	0/1/1/1
10	NAG	K	2	10	-	2/6/23/26	0/1/1/1
10	BMA	K	3	10	-	0/2/19/22	0/1/1/1
10	MAN	K	4	10	-	2/2/19/22	0/1/1/1
10	MAN	K	5	10	-	0/2/19/22	0/1/1/1
10	MAN	K	6	10	-	2/2/19/22	0/1/1/1
10	MAN	K	7	10	-	0/2/19/22	0/1/1/1
10	MAN	K	8	10	-	0/2/19/22	0/1/1/1
10	MAN	K	9	10	-	2/2/19/22	0/1/1/1
9	NAG	M	1	9,4	-	0/6/23/26	0/1/1/1
9	NAG	M	2	9	-	1/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	5	MAN	C1-C2	3.87	1.61	1.52
7	A	5	MAN	O5-C1	3.21	1.48	1.43
7	A	4	MAN	C1-C2	3.11	1.59	1.52
7	A	4	MAN	C2-C3	3.08	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	4	MAN	C1-C2	2.24	1.57	1.52
10	K	9	MAN	C1-C2	2.06	1.56	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	5	MAN	C1-O5-C5	6.77	121.36	112.19
7	A	4	MAN	C1-C2-C3	5.26	116.13	109.67
10	K	9	MAN	C1-O5-C5	4.79	118.69	112.19
10	K	1	NAG	C2-N2-C7	4.53	129.35	122.90
7	A	2	NAG	C2-N2-C7	4.29	129.02	122.90
10	K	4	MAN	C1-O5-C5	3.13	116.44	112.19
10	K	8	MAN	C1-O5-C5	2.85	116.06	112.19
7	A	5	MAN	O5-C1-C2	2.84	115.16	110.77
7	A	5	MAN	C1-C2-C3	2.79	113.09	109.67
7	A	4	MAN	C1-O5-C5	2.73	115.89	112.19
7	A	4	MAN	O5-C1-C2	2.59	114.76	110.77
10	K	1	NAG	C1-C2-N2	2.57	114.88	110.49
7	A	6	MAN	O2-C2-C3	-2.40	105.33	110.14
7	A	6	MAN	C1-O5-C5	2.40	115.44	112.19
10	K	10	MAN	O2-C2-C3	-2.38	105.36	110.14
7	A	4	MAN	C2-C3-C4	2.29	114.86	110.89
10	K	5	MAN	O2-C2-C3	-2.25	105.63	110.14
9	M	1	NAG	C1-O5-C5	2.20	115.17	112.19
10	K	9	MAN	O2-C2-C3	-2.18	105.77	110.14
10	K	4	MAN	O2-C2-C3	-2.17	105.80	110.14
10	K	5	MAN	C1-O5-C5	2.14	115.10	112.19
10	K	7	MAN	O2-C2-C3	-2.12	105.88	110.14
7	A	5	MAN	O2-C2-C3	-2.12	105.89	110.14
10	K	3	BMA	C1-C2-C3	2.11	112.26	109.67
10	K	6	MAN	C1-O5-C5	2.08	115.01	112.19
7	A	4	MAN	O2-C2-C3	-2.01	106.11	110.14

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	2	NAG	O5-C5-C6-O6
10	K	4	MAN	O5-C5-C6-O6
7	A	3	BMA	C4-C5-C6-O6
9	I	1	NAG	O5-C5-C6-O6
9	J	2	NAG	O5-C5-C6-O6

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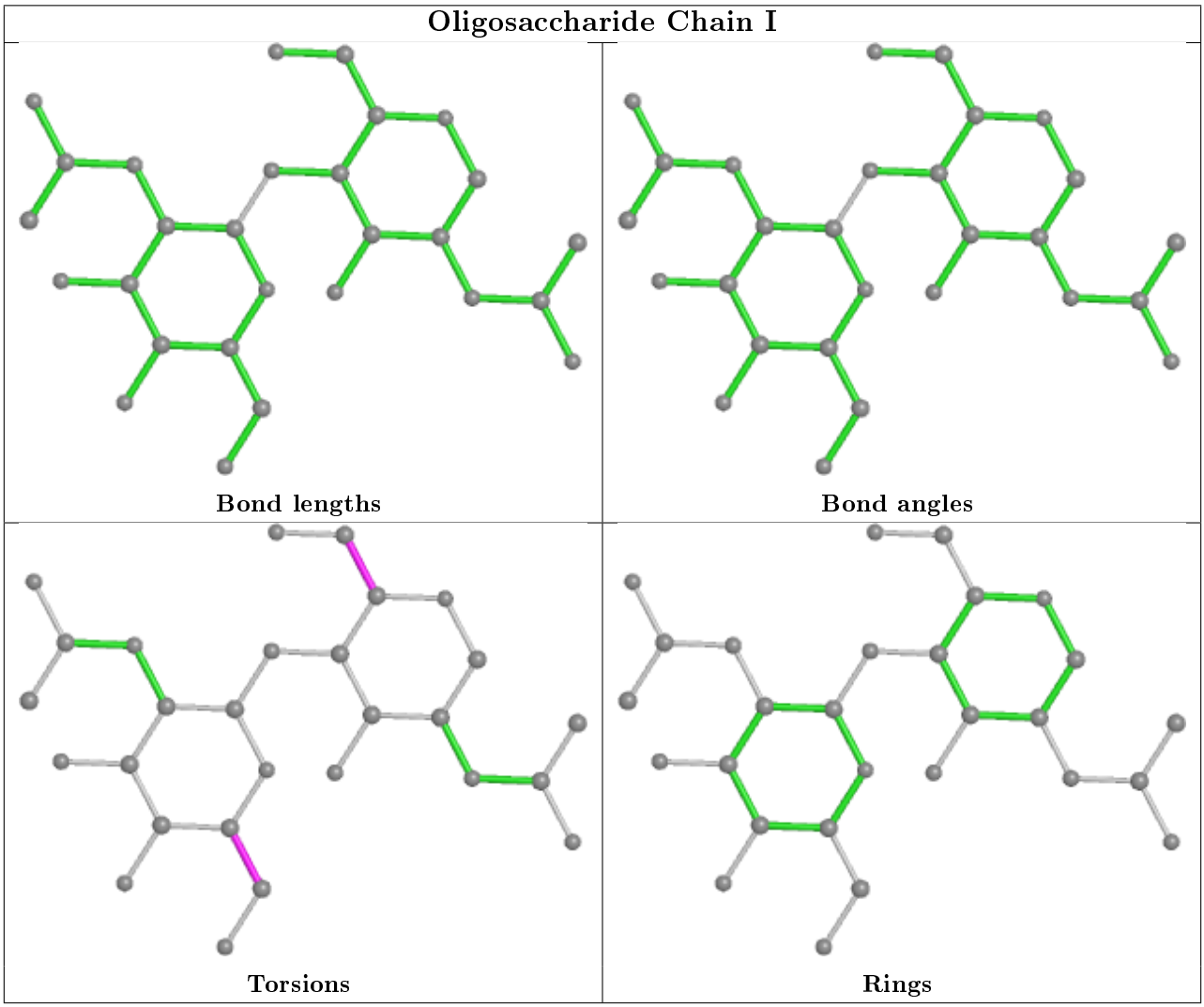
Mol	Chain	Res	Type	Atoms
7	A	3	BMA	O5-C5-C6-O6
9	I	1	NAG	C4-C5-C6-O6
9	J	2	NAG	C4-C5-C6-O6
10	K	9	MAN	O5-C5-C6-O6
10	K	2	NAG	O5-C5-C6-O6
10	K	4	MAN	C4-C5-C6-O6
8	F	2	NAG	C4-C5-C6-O6
10	K	1	NAG	C8-C7-N2-C2
10	K	1	NAG	O7-C7-N2-C2
7	A	2	NAG	C8-C7-N2-C2
7	A	2	NAG	O7-C7-N2-C2
10	K	6	MAN	O5-C5-C6-O6
8	F	1	NAG	O5-C5-C6-O6
10	K	2	NAG	C4-C5-C6-O6
8	F	1	NAG	C4-C5-C6-O6
10	K	9	MAN	C4-C5-C6-O6
7	A	4	MAN	O5-C5-C6-O6
9	M	2	NAG	O5-C5-C6-O6
7	A	2	NAG	C4-C5-C6-O6
9	I	2	NAG	O5-C5-C6-O6
10	K	6	MAN	C4-C5-C6-O6
7	A	2	NAG	O5-C5-C6-O6
7	A	5	MAN	O5-C5-C6-O6
7	A	4	MAN	C4-C5-C6-O6
8	C	1	NAG	C4-C5-C6-O6
9	J	1	NAG	O5-C5-C6-O6
10	K	1	NAG	C3-C2-N2-C7
7	A	2	NAG	C3-C2-N2-C7
10	K	1	NAG	C1-C2-N2-C7

There are no ring outliers.

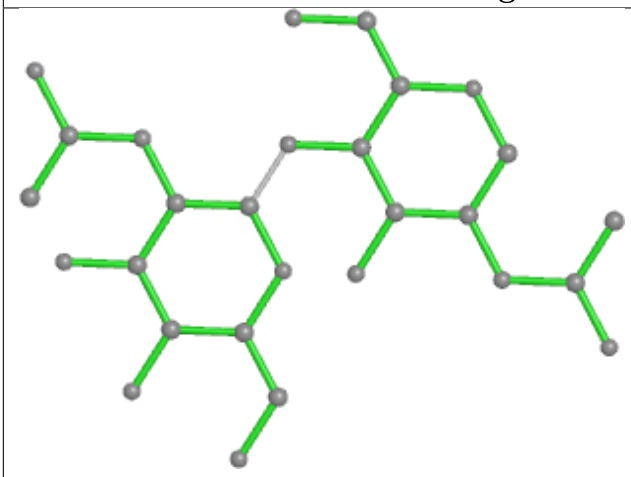
7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	K	1	NAG	1	0
7	A	1	NAG	1	0
10	K	5	MAN	1	0
7	A	2	NAG	1	0
10	K	4	MAN	1	0
7	A	4	MAN	2	0
8	C	1	NAG	1	0

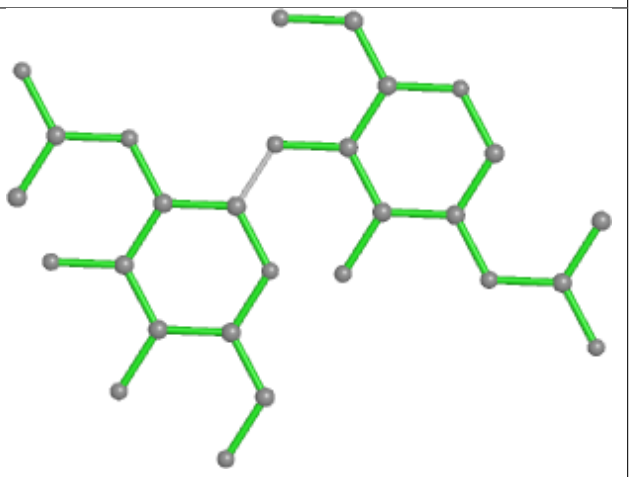
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



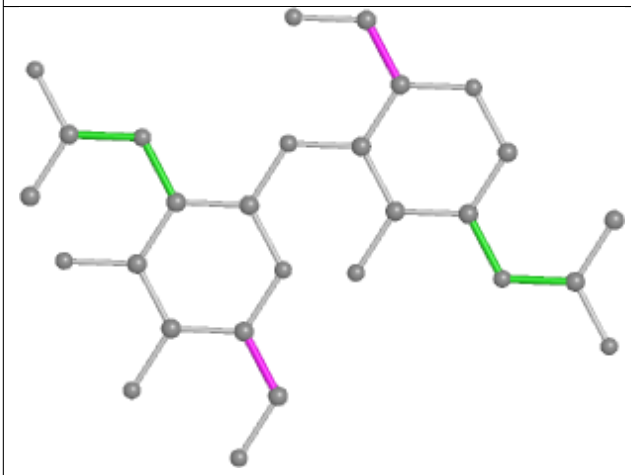
Oligosaccharide Chain J



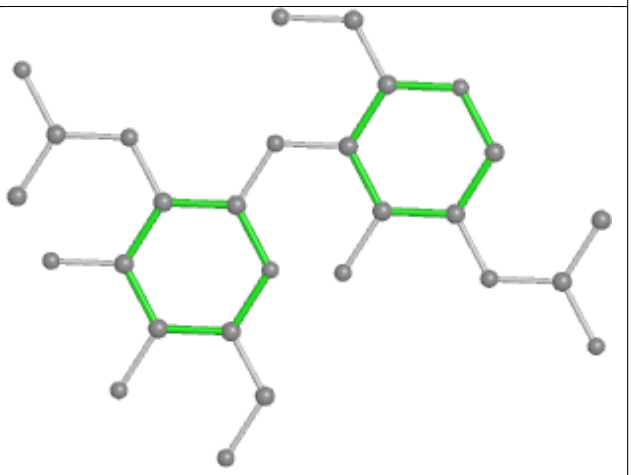
Bond lengths



Bond angles

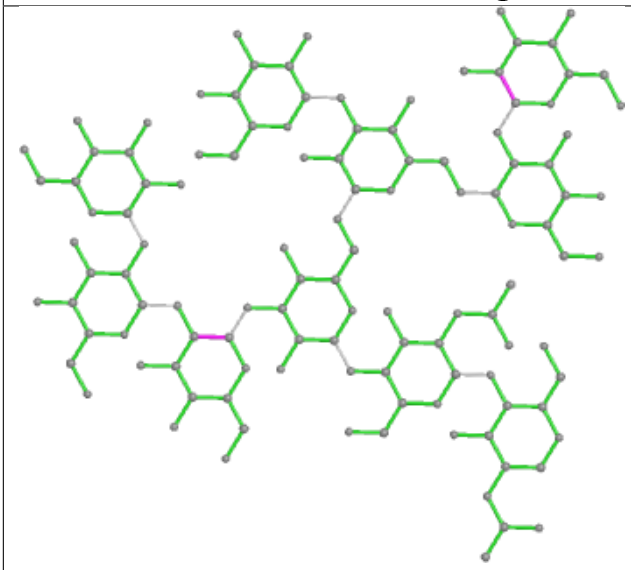


Torsions

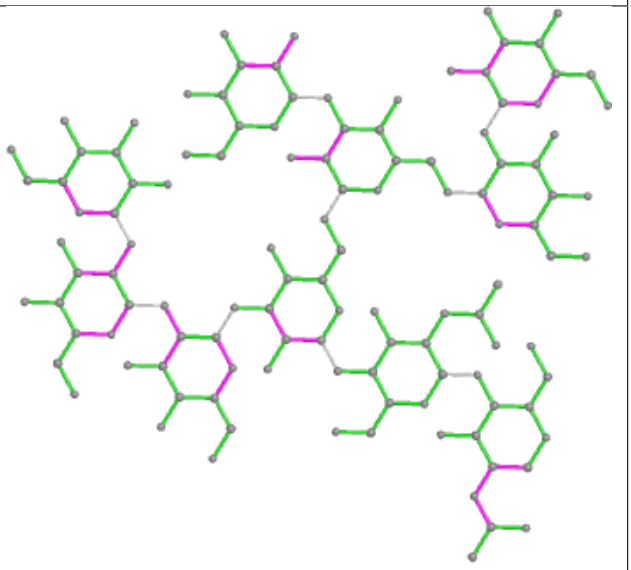


Rings

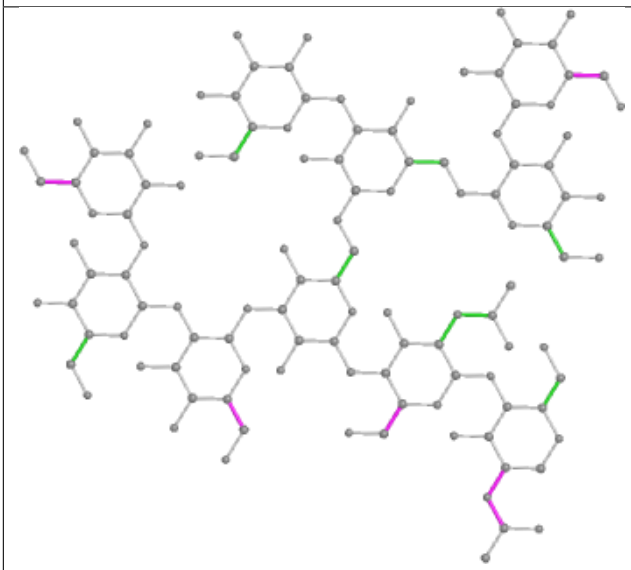
Oligosaccharide Chain K



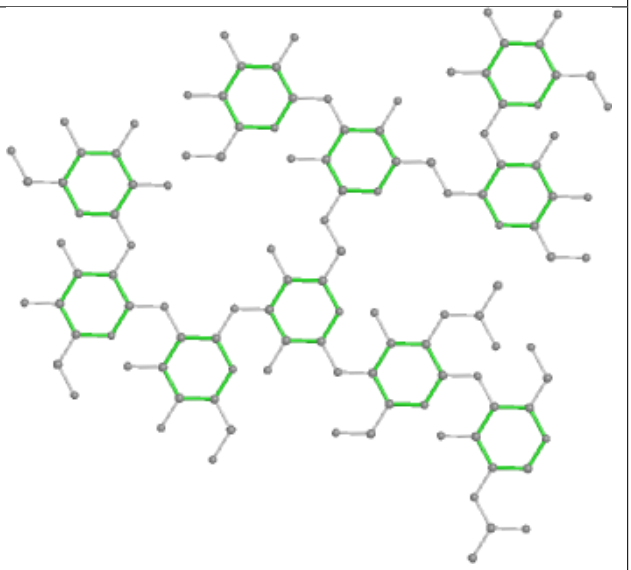
Bond lengths



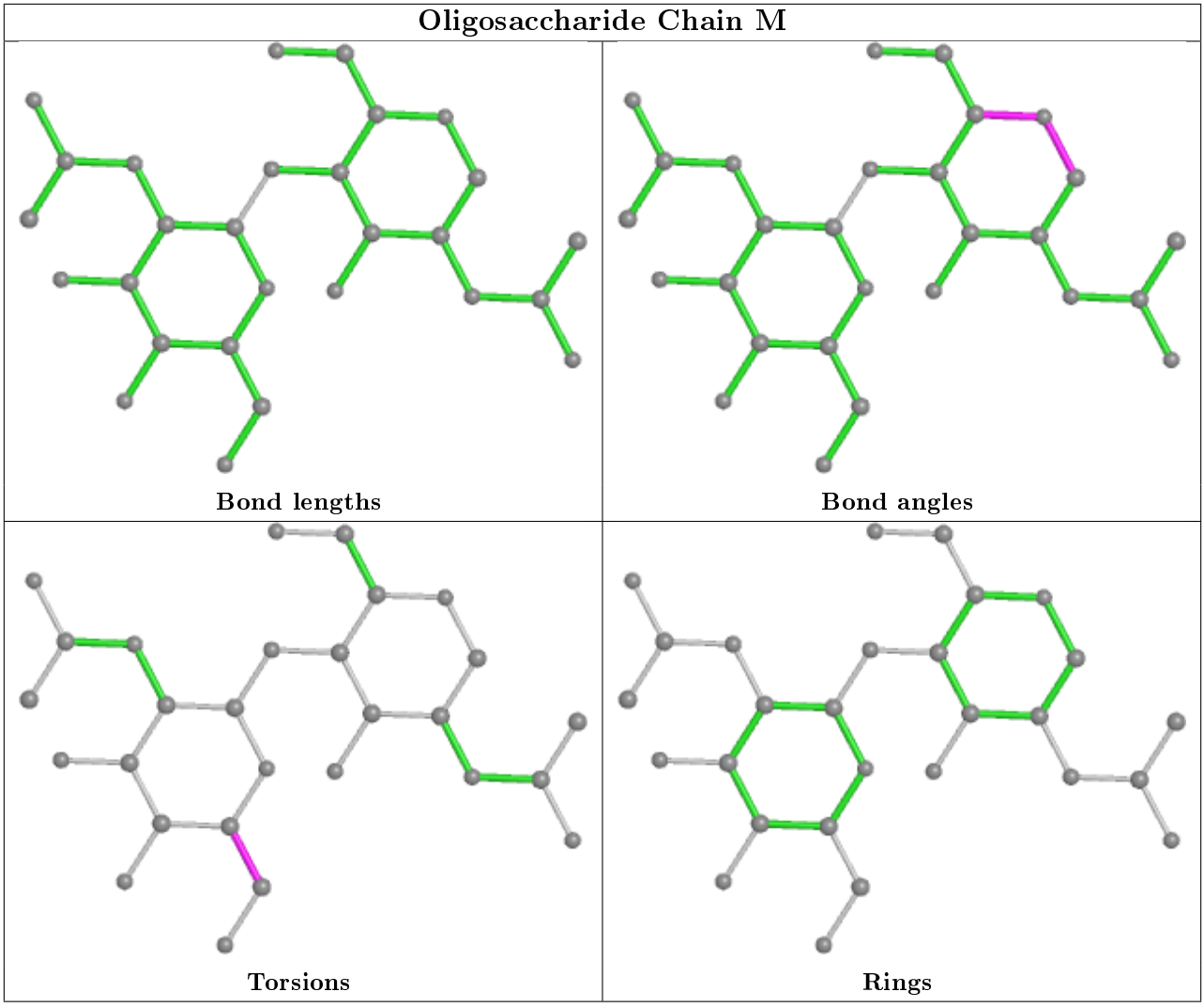
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

13 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	$\#\|Z\| > 2$
11	NAG	B	703	1	14,14,15	0.30	0	17,19,21	0.45	0
11	NAG	B	702	1	14,14,15	0.30	0	17,19,21	0.43	0
11	NAG	G	612	4	14,14,15	0.24	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	JYY	G	637	-	40,45,45	5.45	23 (57%)	45,63,63	2.77	18 (40%)
11	NAG	G	617	4	14,14,15	0.28	0	17,19,21	0.45	0
11	NAG	B	701	1	14,14,15	0.39	0	17,19,21	0.59	0
11	NAG	G	607	4	14,14,15	0.26	0	17,19,21	0.57	0
11	NAG	G	613	4	14,14,15	0.30	0	17,19,21	0.41	0
11	NAG	G	633	4	14,14,15	0.27	0	17,19,21	0.46	0
11	NAG	G	632	4	14,14,15	0.28	0	17,19,21	0.49	0
11	NAG	G	611	4	14,14,15	0.47	0	17,19,21	0.48	0
11	NAG	G	634	4	14,14,15	0.23	0	17,19,21	0.50	0
11	NAG	D	201	2	14,14,15	0.34	0	17,19,21	0.49	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
11	NAG	B	703	1	-	1/6/23/26	0/1/1/1
11	NAG	B	702	1	-	2/6/23/26	0/1/1/1
11	NAG	G	612	4	-	1/6/23/26	0/1/1/1
12	JYY	G	637	-	1/1/6/7	9/23/46/46	0/5/5/5
11	NAG	G	617	4	-	2/6/23/26	0/1/1/1
11	NAG	B	701	1	-	2/6/23/26	0/1/1/1
11	NAG	G	607	4	-	0/6/23/26	0/1/1/1
11	NAG	G	613	4	-	2/6/23/26	0/1/1/1
11	NAG	G	633	4	-	2/6/23/26	0/1/1/1
11	NAG	G	632	4	-	0/6/23/26	0/1/1/1
11	NAG	G	611	4	-	2/6/23/26	0/1/1/1
11	NAG	G	634	4	-	2/6/23/26	0/1/1/1
11	NAG	D	201	2	-	2/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	637	JYY	C01-N30	13.98	1.46	1.32
12	G	637	JYY	C17-S41	-13.86	1.54	1.73
12	G	637	JYY	C16-S41	-11.88	1.51	1.70
12	G	637	JYY	C23-C22	8.69	1.53	1.39
12	G	637	JYY	C27-C22	8.67	1.53	1.39
12	G	637	JYY	C05-C04	7.78	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	637	JYY	C17-N33	7.24	1.41	1.31
12	G	637	JYY	C26-C27	6.63	1.52	1.38
12	G	637	JYY	C24-C23	6.61	1.52	1.38
12	G	637	JYY	C15-N33	6.19	1.56	1.37
12	G	637	JYY	C21-C28	6.04	1.52	1.47
12	G	637	JYY	C09-N32	5.88	1.45	1.34
12	G	637	JYY	C04-C03	5.86	1.55	1.42
12	G	637	JYY	C25-C24	5.67	1.53	1.38
12	G	637	JYY	C26-C25	5.65	1.53	1.38
12	G	637	JYY	C18-N34	5.42	1.45	1.33
12	G	637	JYY	C05-N30	5.05	1.45	1.34
12	G	637	JYY	C01-C15	2.87	1.52	1.50
12	G	637	JYY	C07-C03	-2.37	1.38	1.42
12	G	637	JYY	C07-C08	2.24	1.53	1.49
12	G	637	JYY	C17-C18	2.20	1.53	1.49
12	G	637	JYY	O39-C18	-2.17	1.18	1.23
12	G	637	JYY	O37-C09	-2.01	1.18	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	637	JYY	C11-C12-C21	7.70	123.14	112.09
12	G	637	JYY	C22-C21-C28	6.95	119.58	110.88
12	G	637	JYY	C13-C12-C21	6.75	121.78	112.09
12	G	637	JYY	C10-C11-C12	5.05	119.90	109.29
12	G	637	JYY	C15-C01-N30	4.47	121.79	114.54
12	G	637	JYY	C11-C10-N32	4.18	117.18	110.82
12	G	637	JYY	O40-C04-C03	3.85	121.55	115.89
12	G	637	JYY	C15-C16-S41	-3.71	107.24	111.79
12	G	637	JYY	C15-C01-C02	-3.62	117.20	123.47
12	G	637	JYY	C29-O40-C04	-3.27	113.17	117.75
12	G	637	JYY	O40-C04-C05	-3.16	117.74	125.08
12	G	637	JYY	C06-C07-C08	-3.07	121.92	127.45
12	G	637	JYY	C08-C09-N32	2.71	121.19	118.52
12	G	637	JYY	C11-C12-C13	2.57	113.97	109.44
12	G	637	JYY	C17-C18-N34	2.52	118.11	115.60
12	G	637	JYY	C07-C08-C09	2.44	122.12	118.61
12	G	637	JYY	O37-C09-N32	-2.40	118.84	122.67
12	G	637	JYY	O37-C09-C08	2.03	119.97	116.91

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	G	637	JYY	C21

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	G	637	JYY	C11-C12-C21-C22
12	G	637	JYY	N30-C01-C15-C16
12	G	637	JYY	C03-C04-O40-C29
11	G	633	NAG	C4-C5-C6-O6
11	G	617	NAG	O5-C5-C6-O6
11	G	613	NAG	O5-C5-C6-O6
11	D	201	NAG	O5-C5-C6-O6
11	B	702	NAG	O5-C5-C6-O6
11	G	634	NAG	O5-C5-C6-O6
12	G	637	JYY	C05-C04-O40-C29
11	G	633	NAG	O5-C5-C6-O6
11	G	617	NAG	C4-C5-C6-O6
11	B	701	NAG	O5-C5-C6-O6
11	G	634	NAG	C4-C5-C6-O6
11	B	701	NAG	C4-C5-C6-O6
11	G	613	NAG	C4-C5-C6-O6
11	B	703	NAG	O5-C5-C6-O6
12	G	637	JYY	N34-C19-C20-O38
11	D	201	NAG	C4-C5-C6-O6
11	G	612	NAG	O5-C5-C6-O6
11	G	611	NAG	C4-C5-C6-O6
11	B	702	NAG	C4-C5-C6-O6
11	G	611	NAG	O5-C5-C6-O6
12	G	637	JYY	O36-C08-C09-O37
12	G	637	JYY	C13-C12-C21-C22
12	G	637	JYY	C13-C12-C21-C28
12	G	637	JYY	C11-C12-C21-C28

There are no ring outliers.

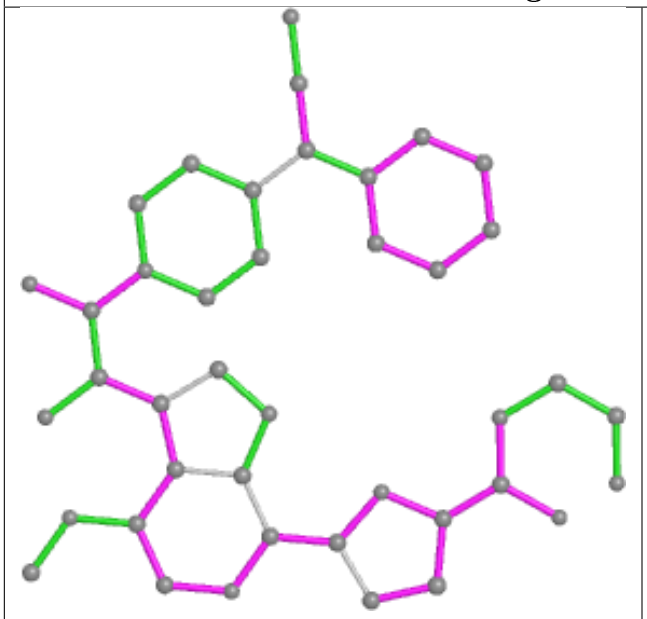
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	637	JYY	1	0
11	G	613	NAG	1	0

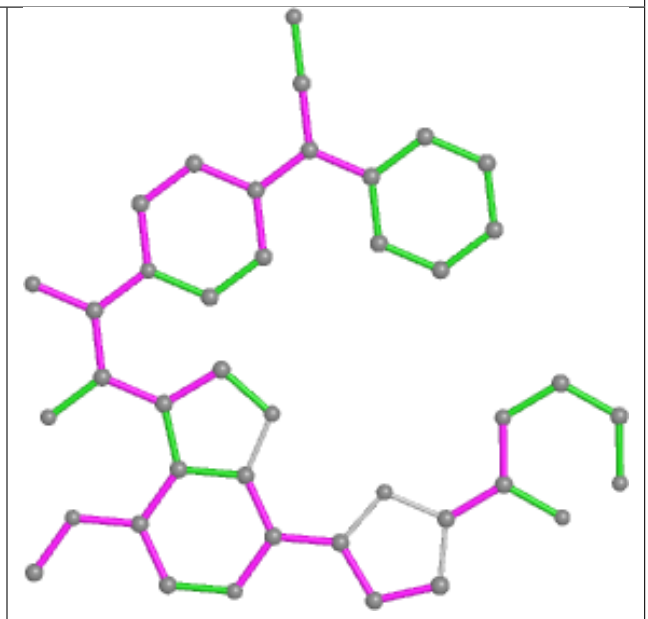
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

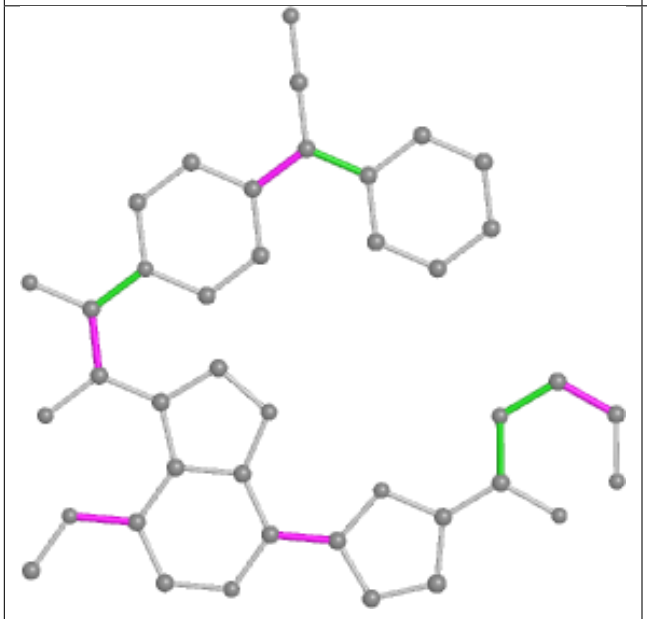
Ligand JYY G 637



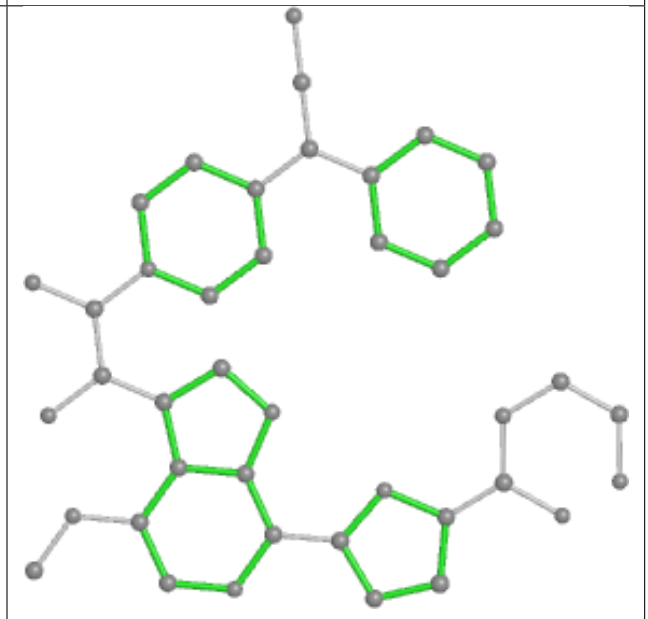
Bond lengths



Bond angles



Torsions



Rings

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	133/153 (86%)	-0.21	4 (3%) 50 53	5, 28, 59, 101	0
2	D	128/134 (95%)	0.42	11 (8%) 10 10	34, 65, 91, 99	0
3	E	105/114 (92%)	0.23	5 (4%) 30 32	32, 56, 86, 98	0
4	G	442/481 (91%)	-0.32	13 (2%) 51 55	6, 24, 72, 104	0
5	H	226/244 (92%)	-0.12	6 (2%) 54 58	14, 43, 76, 96	0
6	L	211/217 (97%)	-0.51	1 (0%) 91 91	10, 28, 47, 99	0
All	All	1245/1343 (92%)	-0.18	40 (3%) 47 51	5, 34, 82, 104	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	517	ALA	9.5
5	H	187	LEU	5.6
2	D	18	VAL	5.1
4	G	396	ILE	5.1
6	L	7	TYR	5.0
1	B	518	VAL	4.7
2	D	110	THR	3.9
4	G	188	ASN	3.8
4	G	79	PRO	3.8
4	G	397	SER	3.6
2	D	42	GLY	3.6
5	H	26	GLY	3.5
5	H	189	THR	3.4
2	D	14	PRO	3.3
4	G	138	ILE	3.2
4	G	141	ASP	3.2
1	B	548	ILE	3.2
3	E	8	ALA	3.0
3	E	16	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
4	G	358	ILE	2.8
2	D	8	GLY	2.8
5	H	125	SER	2.7
3	E	103	LYS	2.7
4	G	356	ASN	2.7
5	H	30	SER	2.7
3	E	15	LEU	2.7
4	G	410	SER	2.6
4	G	78	ASP	2.4
4	G	398	ASN	2.2
2	D	109	LEU	2.2
1	B	519	PHE	2.2
2	D	64	GLN	2.2
5	H	183	PRO	2.2
4	G	80	ASN	2.1
2	D	11	THR	2.1
3	E	18	SER	2.1
2	D	5	VAL	2.1
2	D	89	THR	2.1
2	D	84	SER	2.1
4	G	409	GLY	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, 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
8	BMA	F	3	11/12	0.86	0.27	88,99,104,104	0
10	MAN	K	9	11/12	0.87	0.29	59,79,95,95	0
9	NAG	I	2	14/15	0.87	0.29	71,80,103,107	0
7	MAN	A	5	11/12	0.88	0.21	70,76,97,101	0
7	MAN	A	4	11/12	0.88	0.17	55,64,80,80	0
9	NAG	M	2	14/15	0.89	0.18	63,85,103,104	0
8	BMA	C	3	11/12	0.89	0.20	69,90,98,100	0

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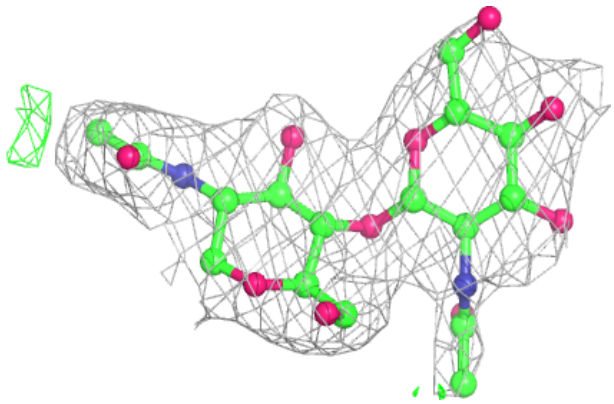
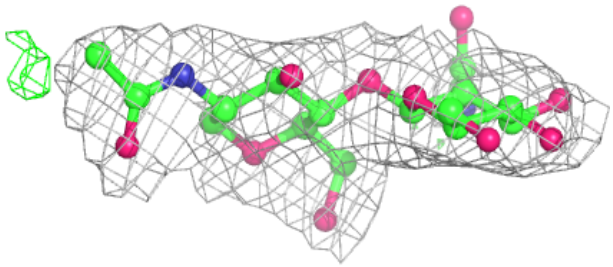
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	J	2	14/15	0.90	0.21	39,63,80,83	0
8	NAG	F	2	14/15	0.90	0.17	32,50,82,94	0
10	MAN	K	10	11/12	0.92	0.14	52,62,74,74	0
9	NAG	M	1	14/15	0.93	0.14	32,52,79,80	0
10	MAN	K	6	11/12	0.93	0.12	20,30,42,46	0
10	MAN	K	8	11/12	0.94	0.13	38,52,69,73	0
10	NAG	K	1	14/15	0.94	0.14	24,39,53,54	0
8	NAG	C	2	14/15	0.95	0.12	32,61,83,85	0
10	MAN	K	7	11/12	0.95	0.09	38,48,56,72	0
7	NAG	A	2	14/15	0.96	0.10	22,30,36,56	0
8	NAG	C	1	14/15	0.96	0.11	19,34,53,59	0
7	NAG	A	1	14/15	0.96	0.12	17,24,29,32	0
7	BMA	A	3	11/12	0.96	0.10	23,30,42,47	0
10	NAG	K	2	14/15	0.97	0.10	6,37,51,53	0
10	MAN	K	4	11/12	0.97	0.11	12,16,24,37	0
7	MAN	A	6	11/12	0.97	0.09	15,29,41,47	0
8	NAG	F	1	14/15	0.97	0.14	4,18,28,38	0
9	NAG	J	1	14/15	0.97	0.12	19,27,43,54	0
9	NAG	I	1	14/15	0.97	0.09	29,40,57,72	0
10	MAN	K	5	11/12	0.97	0.11	15,17,28,30	0
10	BMA	K	3	11/12	0.97	0.08	19,27,33,47	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:

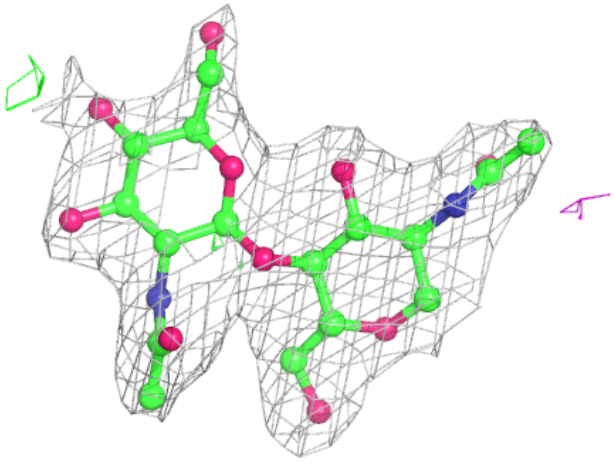
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

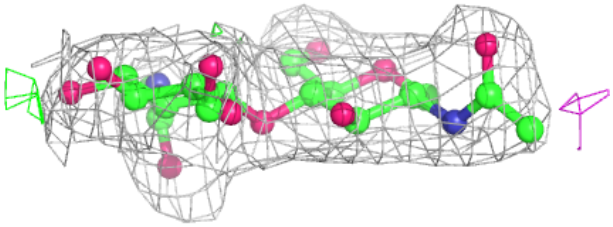


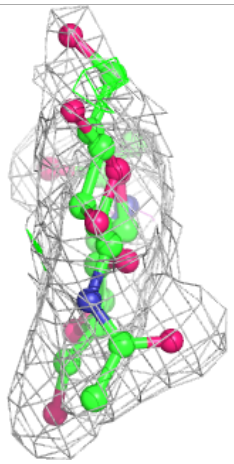


Electron density around Chain J:

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

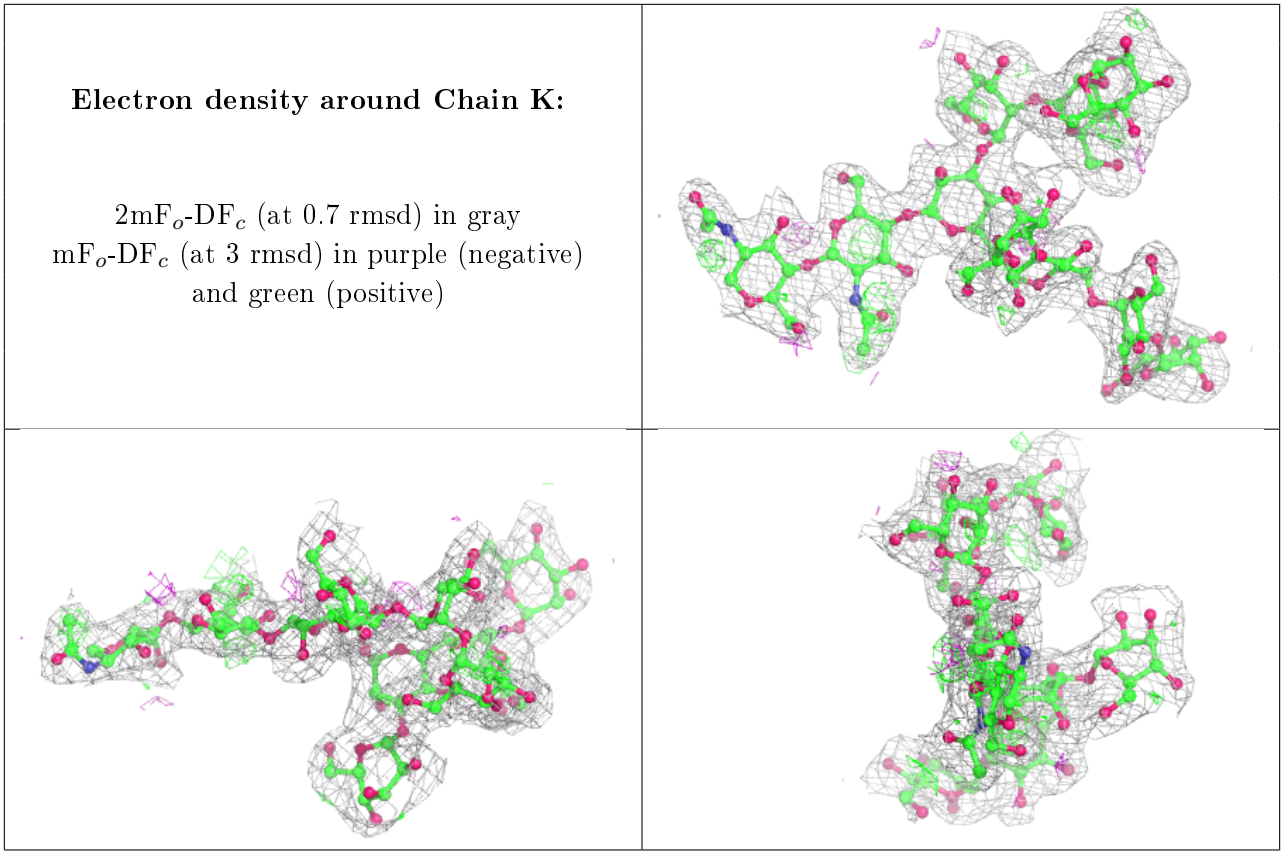






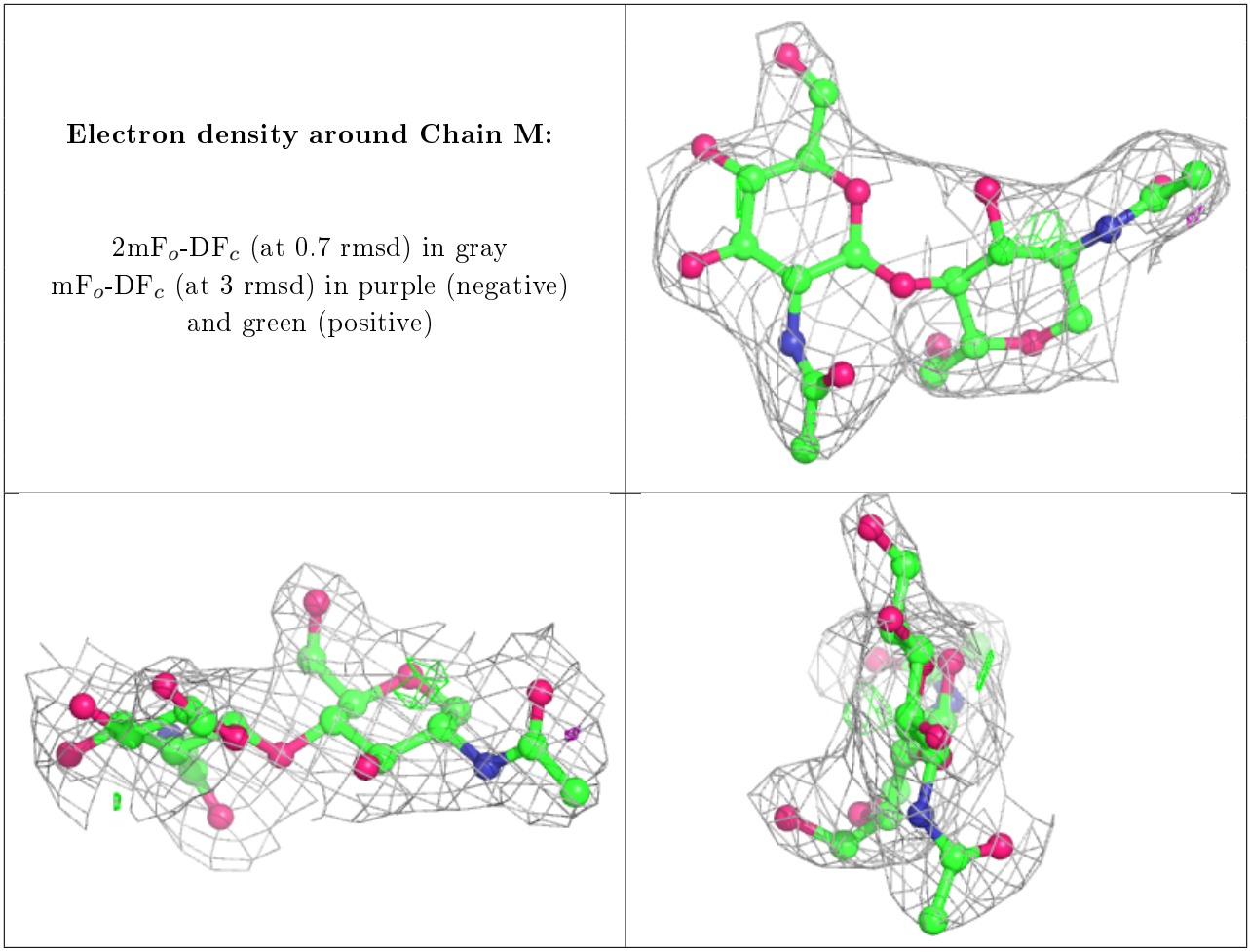
Electron density around Chain K:

$2mF_o$-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 M:

$2mF_o$-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
11	NAG	B	703	14/15	0.88	0.27	54,81,90,93	0
11	NAG	G	632	14/15	0.88	0.29	65,77,84,88	0
11	NAG	B	701	14/15	0.90	0.40	63,86,99,104	0
11	NAG	G	617	14/15	0.91	0.25	50,73,95,95	0
11	NAG	D	201	14/15	0.91	0.23	52,76,86,89	0
11	NAG	G	612	14/15	0.92	0.16	36,61,67,71	0
11	NAG	G	633	14/15	0.93	0.15	43,51,58,67	0
11	NAG	B	702	14/15	0.93	0.36	68,80,91,102	0
11	NAG	G	613	14/15	0.93	0.12	56,65,77,79	0
11	NAG	G	607	14/15	0.94	0.16	43,54,82,86	0
11	NAG	G	634	14/15	0.95	0.13	25,39,49,52	0

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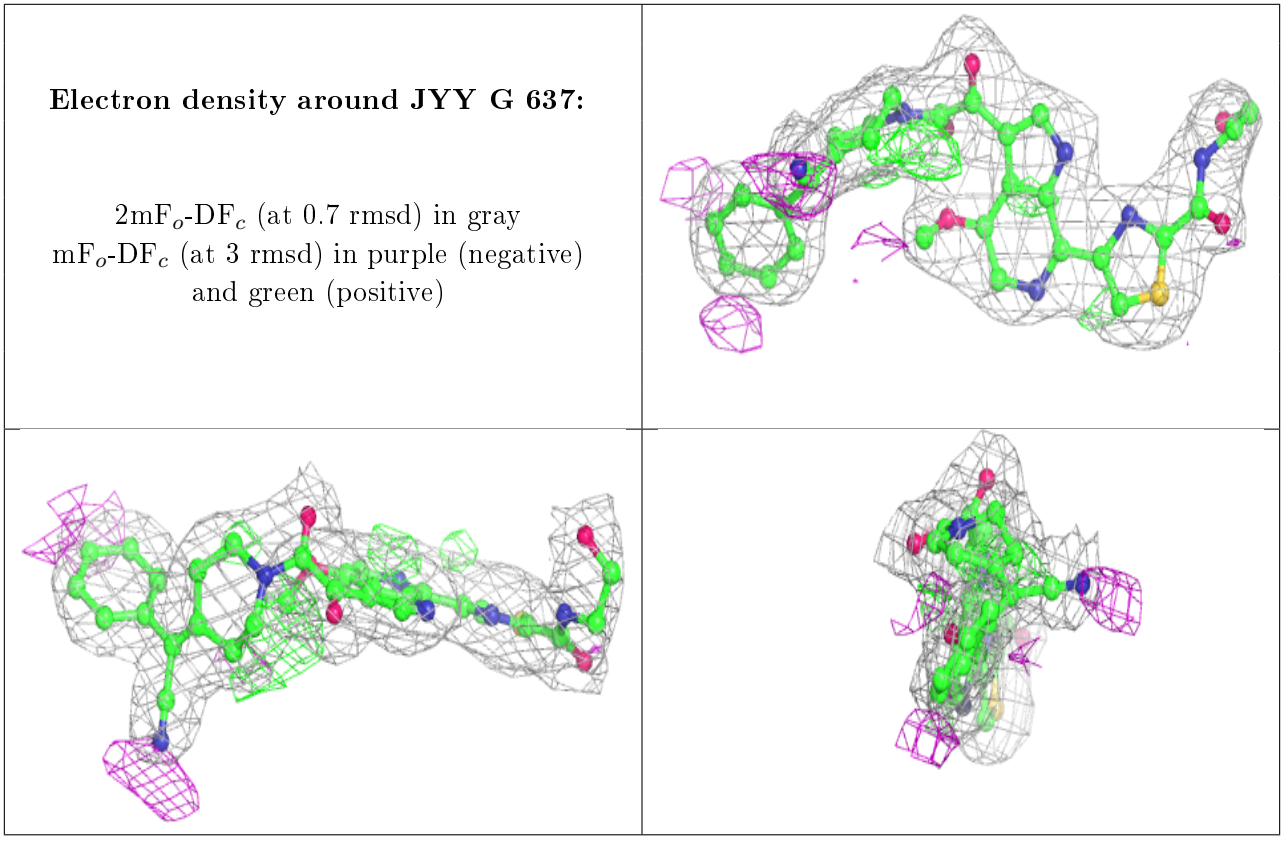
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	NAG	G	611	14/15	0.95	0.12	20,40,51,52	0
12	JYY	G	637	41/41	0.96	0.13	3,16,36,51	0

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 JYY G 637:

$2mF_o$-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.