Full wwPDB X-ray Structure Validation Report (i)

Aug 10, 2020 – 01:19 PM BST

PDB ID	:	4ADF
Title	:	CRYSTAL STRUCTURE OF THE HUMAN COLONY-STIMULATING FACTOR 1 (hCSF-1) CYTOKINE IN COMPLEX WITH THE VIRAL RECEPTOR BARF1
Authors	:	Elegheert, J.; Bracke, N.; Savvides, S.N.
Deposited on	:	2011-12-23
Resolution	:	4.40 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 following versions of software and data (see references (1)) were used in the production of this report:

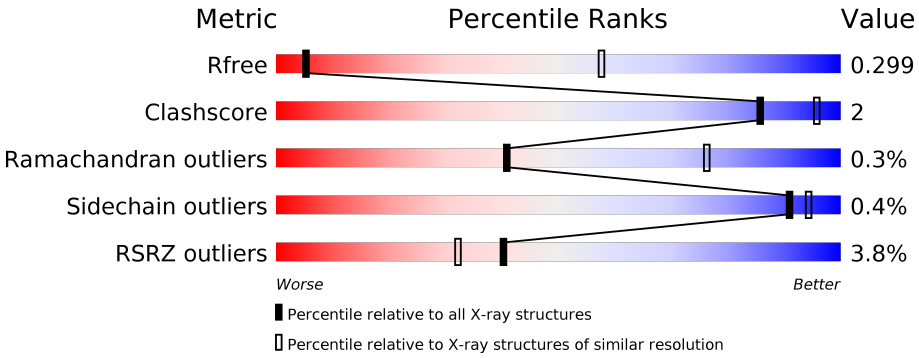
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 4.40 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	1043 (5.00-3.80)
Clashscore	141614	1111 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)
RSRZ outliers	127900	1095 (5.08-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	208	88% · 10%
1	B	208	2% 88% · 9%
1	C	208	9% 86% · 11%
1	D	208	2% 89% · 10%
1	E	208	12% 86% · 10%
1	F	208	3% 87% · 9%

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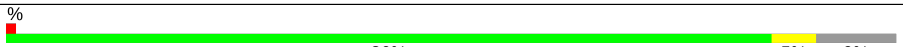
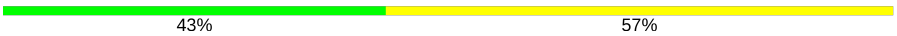
Mol	Chain	Length	Quality of chain
1	M	208	
1	N	208	
1	O	208	
1	P	208	
1	Q	208	
1	R	208	
2	G	153	
2	H	153	
2	I	153	
2	J	153	
2	K	153	
2	L	153	
2	S	153	
2	T	153	
2	U	153	
2	V	153	
2	W	153	
2	X	153	
3	Y	6	
3	e	6	
3	f	6	
3	h	6	
4	Z	7	
4	a	7	
4	i	7	

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Mol	Chain	Length	Quality of chain
4	j	7	100%
5	b	5	100%
5	c	5	20% 80%
5	d	5	20% 80%
5	g	5	20% 80%

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
4	MAN	a	4	-	-	-	X
4	MAN	a	5	-	-	-	X
4	MAN	a	6	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32413 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 SECRETED PROTEIN BARF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1494	965	255	267	7			
1	B	189	Total	C	N	O	S	0	0	0
			1498	967	255	269	7			
1	C	186	Total	C	N	O	S	0	0	0
			1481	956	253	265	7			
1	D	187	Total	C	N	O	S	0	0	0
			1487	960	253	267	7			
1	E	187	Total	C	N	O	S	0	0	0
			1485	959	253	266	7			
1	F	189	Total	C	N	O	S	0	0	0
			1495	965	255	268	7			
1	M	191	Total	C	N	O	S	0	0	0
			1507	973	257	270	7			
1	N	191	Total	C	N	O	S	0	0	0
			1517	978	259	273	7			
1	O	186	Total	C	N	O	S	0	0	0
			1476	954	250	265	7			
1	P	189	Total	C	N	O	S	0	0	0
			1502	970	256	269	7			
1	Q	185	Total	C	N	O	S	0	0	0
			1481	958	252	264	7			
1	R	186	Total	C	N	O	S	0	0	0
			1483	958	252	266	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	LYS	-	expression tag	UNP P0CW72
A	223	HIS	-	expression tag	UNP P0CW72
A	224	HIS	-	expression tag	UNP P0CW72
A	225	HIS	-	expression tag	UNP P0CW72
A	226	HIS	-	expression tag	UNP P0CW72

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Chain	Residue	Modelled	Actual	Comment	Reference
A	227	HIS	-	expression tag	UNP P0CW72
A	228	HIS	-	expression tag	UNP P0CW72
A	169	SER	THR	engineered mutation	UNP P0CW72
B	222	LYS	-	expression tag	UNP P0CW72
B	223	HIS	-	expression tag	UNP P0CW72
B	224	HIS	-	expression tag	UNP P0CW72
B	225	HIS	-	expression tag	UNP P0CW72
B	226	HIS	-	expression tag	UNP P0CW72
B	227	HIS	-	expression tag	UNP P0CW72
B	228	HIS	-	expression tag	UNP P0CW72
B	169	SER	THR	engineered mutation	UNP P0CW72
C	222	LYS	-	expression tag	UNP P0CW72
C	223	HIS	-	expression tag	UNP P0CW72
C	224	HIS	-	expression tag	UNP P0CW72
C	225	HIS	-	expression tag	UNP P0CW72
C	226	HIS	-	expression tag	UNP P0CW72
C	227	HIS	-	expression tag	UNP P0CW72
C	228	HIS	-	expression tag	UNP P0CW72
C	169	SER	THR	engineered mutation	UNP P0CW72
D	222	LYS	-	expression tag	UNP P0CW72
D	223	HIS	-	expression tag	UNP P0CW72
D	224	HIS	-	expression tag	UNP P0CW72
D	225	HIS	-	expression tag	UNP P0CW72
D	226	HIS	-	expression tag	UNP P0CW72
D	227	HIS	-	expression tag	UNP P0CW72
D	228	HIS	-	expression tag	UNP P0CW72
D	169	SER	THR	engineered mutation	UNP P0CW72
E	222	LYS	-	expression tag	UNP P0CW72
E	223	HIS	-	expression tag	UNP P0CW72
E	224	HIS	-	expression tag	UNP P0CW72
E	225	HIS	-	expression tag	UNP P0CW72
E	226	HIS	-	expression tag	UNP P0CW72
E	227	HIS	-	expression tag	UNP P0CW72
E	228	HIS	-	expression tag	UNP P0CW72
E	169	SER	THR	engineered mutation	UNP P0CW72
F	222	LYS	-	expression tag	UNP P0CW72
F	223	HIS	-	expression tag	UNP P0CW72
F	224	HIS	-	expression tag	UNP P0CW72
F	225	HIS	-	expression tag	UNP P0CW72
F	226	HIS	-	expression tag	UNP P0CW72
F	227	HIS	-	expression tag	UNP P0CW72
F	228	HIS	-	expression tag	UNP P0CW72

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Chain	Residue	Modelled	Actual	Comment	Reference
F	169	SER	THR	engineered mutation	UNP P0CW72
M	222	LYS	-	expression tag	UNP P0CW72
M	223	HIS	-	expression tag	UNP P0CW72
M	224	HIS	-	expression tag	UNP P0CW72
M	225	HIS	-	expression tag	UNP P0CW72
M	226	HIS	-	expression tag	UNP P0CW72
M	227	HIS	-	expression tag	UNP P0CW72
M	228	HIS	-	expression tag	UNP P0CW72
M	169	SER	THR	engineered mutation	UNP P0CW72
N	222	LYS	-	expression tag	UNP P0CW72
N	223	HIS	-	expression tag	UNP P0CW72
N	224	HIS	-	expression tag	UNP P0CW72
N	225	HIS	-	expression tag	UNP P0CW72
N	226	HIS	-	expression tag	UNP P0CW72
N	227	HIS	-	expression tag	UNP P0CW72
N	228	HIS	-	expression tag	UNP P0CW72
N	169	SER	THR	engineered mutation	UNP P0CW72
O	222	LYS	-	expression tag	UNP P0CW72
O	223	HIS	-	expression tag	UNP P0CW72
O	224	HIS	-	expression tag	UNP P0CW72
O	225	HIS	-	expression tag	UNP P0CW72
O	226	HIS	-	expression tag	UNP P0CW72
O	227	HIS	-	expression tag	UNP P0CW72
O	228	HIS	-	expression tag	UNP P0CW72
O	169	SER	THR	engineered mutation	UNP P0CW72
P	222	LYS	-	expression tag	UNP P0CW72
P	223	HIS	-	expression tag	UNP P0CW72
P	224	HIS	-	expression tag	UNP P0CW72
P	225	HIS	-	expression tag	UNP P0CW72
P	226	HIS	-	expression tag	UNP P0CW72
P	227	HIS	-	expression tag	UNP P0CW72
P	228	HIS	-	expression tag	UNP P0CW72
P	169	SER	THR	engineered mutation	UNP P0CW72
Q	222	LYS	-	expression tag	UNP P0CW72
Q	223	HIS	-	expression tag	UNP P0CW72
Q	224	HIS	-	expression tag	UNP P0CW72
Q	225	HIS	-	expression tag	UNP P0CW72
Q	226	HIS	-	expression tag	UNP P0CW72
Q	227	HIS	-	expression tag	UNP P0CW72
Q	228	HIS	-	expression tag	UNP P0CW72
Q	169	SER	THR	engineered mutation	UNP P0CW72
R	222	LYS	-	expression tag	UNP P0CW72

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Chain	Residue	Modelled	Actual	Comment	Reference
R	223	HIS	-	expression tag	UNP P0CW72
R	224	HIS	-	expression tag	UNP P0CW72
R	225	HIS	-	expression tag	UNP P0CW72
R	226	HIS	-	expression tag	UNP P0CW72
R	227	HIS	-	expression tag	UNP P0CW72
R	228	HIS	-	expression tag	UNP P0CW72
R	169	SER	THR	engineered mutation	UNP P0CW72

- Molecule 2 is a protein called MACROPHAGE COLONY-STIMULATING FACTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	145	Total	C	N	O	S	0	0	0
			1161	729	193	228	11			
2	H	142	Total	C	N	O	S	0	0	0
			1145	722	192	220	11			
2	I	137	Total	C	N	O	S	0	0	0
			1097	690	182	214	11			
2	J	142	Total	C	N	O	S	0	0	0
			1149	723	192	223	11			
2	K	143	Total	C	N	O	S	0	0	0
			1157	726	193	227	11			
2	L	135	Total	C	N	O	S	0	0	0
			1089	686	183	209	11			
2	S	144	Total	C	N	O	S	0	0	0
			1157	726	190	230	11			
2	T	142	Total	C	N	O	S	0	0	0
			1148	723	191	223	11			
2	U	144	Total	C	N	O	S	0	0	0
			1159	727	194	227	11			
2	V	141	Total	C	N	O	S	0	0	0
			1140	719	192	218	11			
2	W	142	Total	C	N	O	S	0	0	0
			1128	710	188	219	11			
2	X	139	Total	C	N	O	S	0	0	0
			1113	702	183	217	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	expression tag	UNP P09603
G	-2	SER	-	expression tag	UNP P09603
G	-1	HIS	-	expression tag	UNP P09603

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	MET	-	expression tag	UNP P09603
H	-3	GLY	-	expression tag	UNP P09603
H	-2	SER	-	expression tag	UNP P09603
H	-1	HIS	-	expression tag	UNP P09603
H	0	MET	-	expression tag	UNP P09603
I	-3	GLY	-	expression tag	UNP P09603
I	-2	SER	-	expression tag	UNP P09603
I	-1	HIS	-	expression tag	UNP P09603
I	0	MET	-	expression tag	UNP P09603
J	-3	GLY	-	expression tag	UNP P09603
J	-2	SER	-	expression tag	UNP P09603
J	-1	HIS	-	expression tag	UNP P09603
J	0	MET	-	expression tag	UNP P09603
K	-3	GLY	-	expression tag	UNP P09603
K	-2	SER	-	expression tag	UNP P09603
K	-1	HIS	-	expression tag	UNP P09603
K	0	MET	-	expression tag	UNP P09603
L	-3	GLY	-	expression tag	UNP P09603
L	-2	SER	-	expression tag	UNP P09603
L	-1	HIS	-	expression tag	UNP P09603
L	0	MET	-	expression tag	UNP P09603
S	-3	GLY	-	expression tag	UNP P09603
S	-2	SER	-	expression tag	UNP P09603
S	-1	HIS	-	expression tag	UNP P09603
S	0	MET	-	expression tag	UNP P09603
T	-3	GLY	-	expression tag	UNP P09603
T	-2	SER	-	expression tag	UNP P09603
T	-1	HIS	-	expression tag	UNP P09603
T	0	MET	-	expression tag	UNP P09603
U	-3	GLY	-	expression tag	UNP P09603
U	-2	SER	-	expression tag	UNP P09603
U	-1	HIS	-	expression tag	UNP P09603
U	0	MET	-	expression tag	UNP P09603
V	-3	GLY	-	expression tag	UNP P09603
V	-2	SER	-	expression tag	UNP P09603
V	-1	HIS	-	expression tag	UNP P09603
V	0	MET	-	expression tag	UNP P09603
W	-3	GLY	-	expression tag	UNP P09603
W	-2	SER	-	expression tag	UNP P09603
W	-1	HIS	-	expression tag	UNP P09603
W	0	MET	-	expression tag	UNP P09603
X	-3	GLY	-	expression tag	UNP P09603

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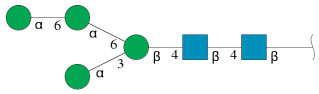
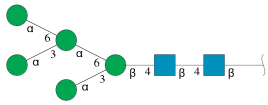
Chain	Residue	Modelled	Actual	Comment	Reference
X	-2	SER	-	expression tag	UNP P09603
X	-1	HIS	-	expression tag	UNP P09603
X	0	MET	-	expression tag	UNP P09603

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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
3	Y	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	e	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	f	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	h	6	Total	C	N	O	0	0	0
			72	40	2	30			

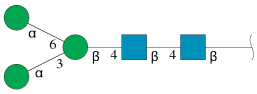
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Z	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	a	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	i	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	j	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran

ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



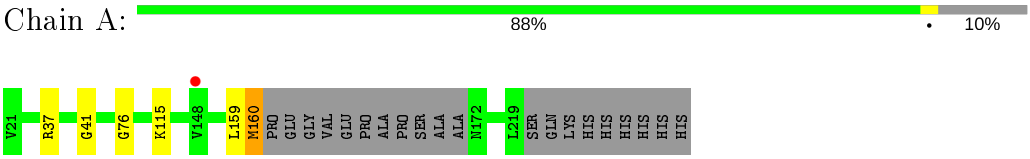
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	b	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	c	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	d	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	g	5	Total	C	N	O	0	0	0
			61	34	2	25			

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.

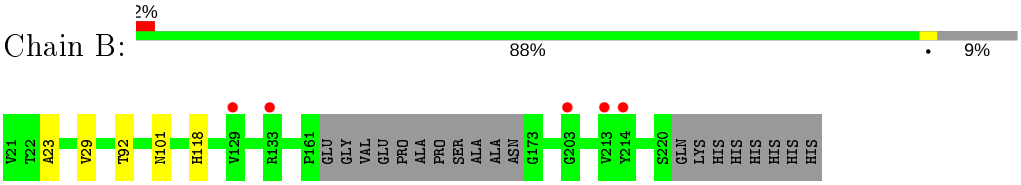
- Molecule 1: SECRETED PROTEIN BARF1

Chain A:



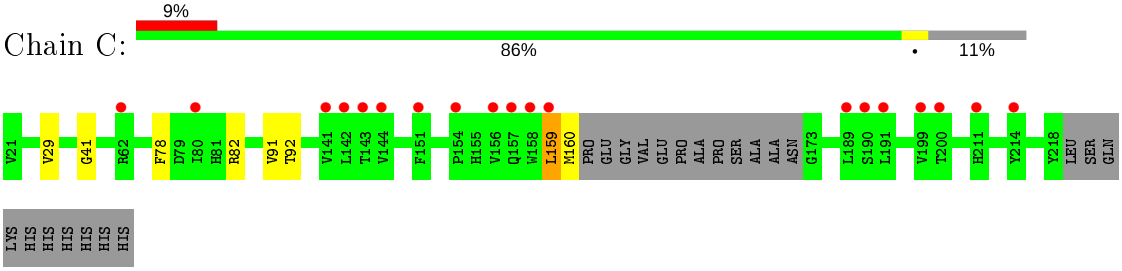
- Molecule 1: SECRETED PROTEIN BARF1

Chain B:



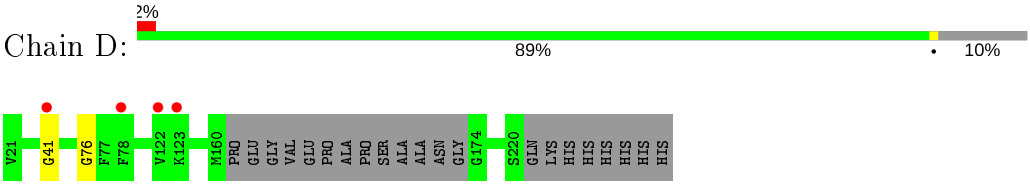
- Molecule 1: SECRETED PROTEIN BARF1

Chain C:



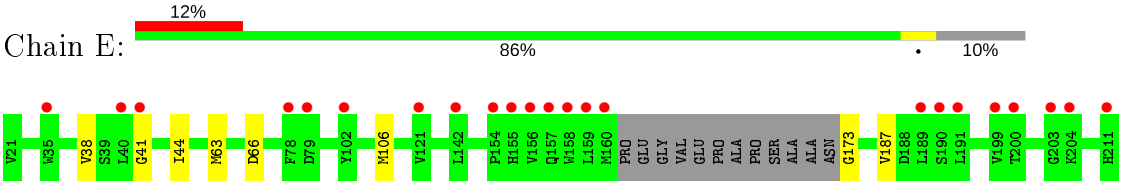
- Molecule 1: SECRETED PROTEIN BARF1

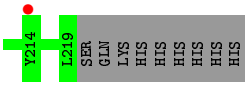
Chain D:



- Molecule 1: SECRETED PROTEIN BARF1

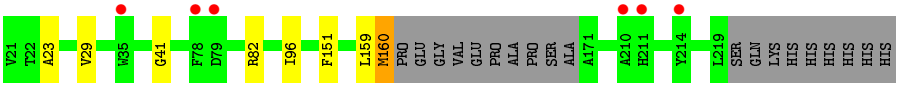
Chain E:





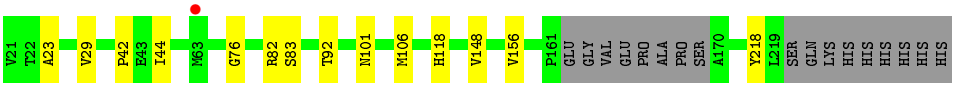
• Molecule 1: SECRETED PROTEIN BARF1

Chain F:



• Molecule 1: SECRETED PROTEIN BARF1

Chain M:



• Molecule 1: SECRETED PROTEIN BARF1

Chain N:

• Molecule 1: SECRETED PROTEIN BARF1

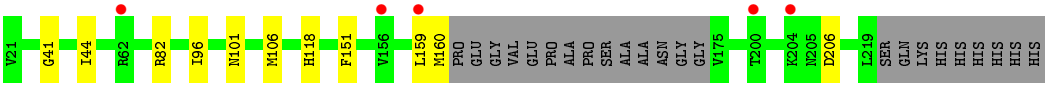
Chain O:

• Molecule 1: SECRETED PROTEIN BARF1

Chain P:

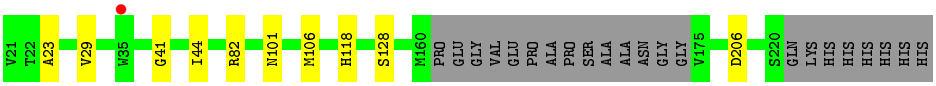
• Molecule 1: SECRETED PROTEIN BARF1

Chain Q:



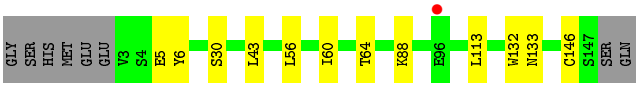
• Molecule 1: SECRETED PROTEIN BARF1

Chain R:



• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain G:



• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

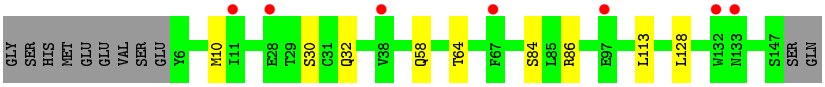
Chain H:

• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain I:

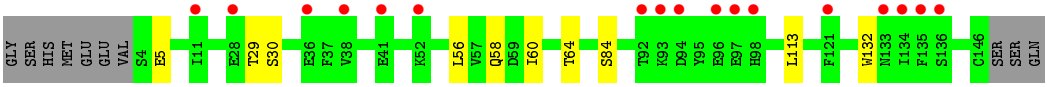
• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain J:



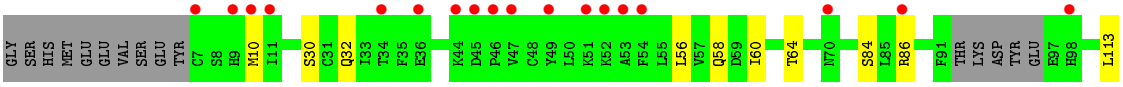
• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

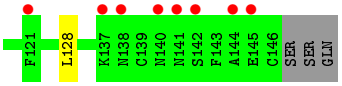
Chain K:



• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

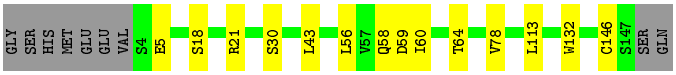
Chain L:





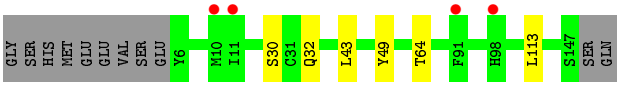
• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain S:



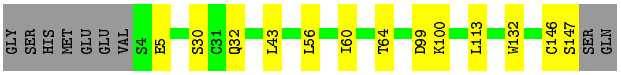
• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain T:



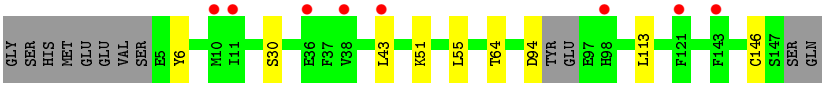
• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain U:



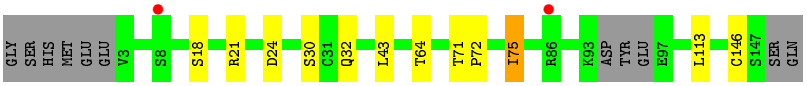
• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain V:



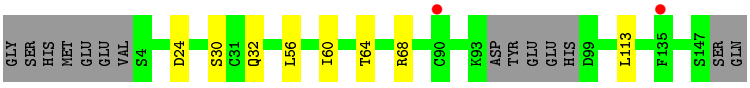
• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain W:



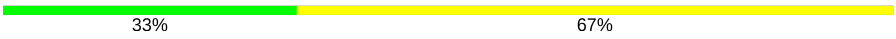
• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

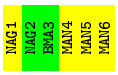
Chain X:



• Molecule 3: alpha-D-mannopyranose-(1-6)-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

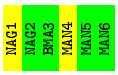
Chain Y:





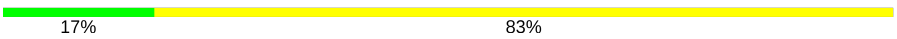
• Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

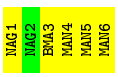
Chain e:



• Molecule 3: alpha-D-mannopyranose-(1-6)-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

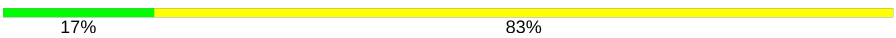
Chain f:

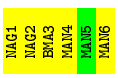




• Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

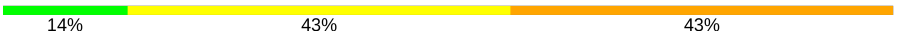
Chain h:





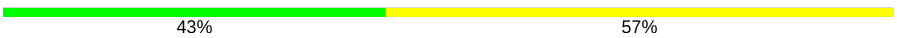
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

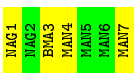
Chain Z:



• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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

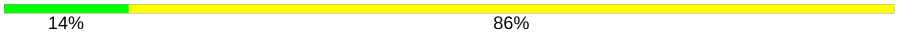
Chain a:





• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 i:

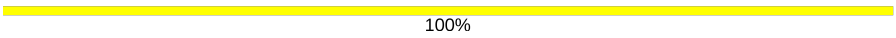


• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:

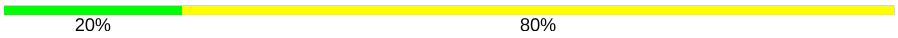
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



• Molecule 5: 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 c:

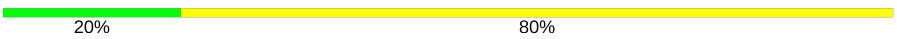


• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

• Molecule 5: 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 g:



NAG1
NAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	218.44Å 218.44Å 331.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.85 – 4.40 75.85 – 4.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (75.85-4.40) 99.2 (75.85-4.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 4.46Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.238 , 0.276 0.275 , 0.299	Depositor DCC
R_{free} test set	2874 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	165.8	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 182.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	32413	wwPDB-VP
Average B, all atoms (Å^2)	216.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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, 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	A	0.31	0/1537	0.65	2/2090 (0.1%)
1	B	0.30	0/1542	0.57	0/2099
1	C	0.31	0/1524	0.60	1/2072 (0.0%)
1	D	0.30	0/1530	0.58	0/2082
1	E	0.30	0/1528	0.56	0/2079
1	F	0.34	0/1538	0.63	1/2093 (0.0%)
1	M	0.33	0/1551	0.63	0/2112
1	N	0.33	0/1561	0.63	0/2123
1	O	0.31	0/1520	0.62	0/2073
1	P	0.32	0/1546	0.58	0/2103
1	Q	0.31	0/1524	0.60	0/2073
1	R	0.32	0/1526	0.61	0/2077
2	G	0.33	0/1179	0.66	0/1591
2	H	0.35	0/1164	0.67	0/1568
2	I	0.31	0/1113	0.63	0/1500
2	J	0.31	0/1168	0.61	1/1574 (0.1%)
2	K	0.30	0/1176	0.58	0/1586
2	L	0.32	0/1106	0.63	1/1490 (0.1%)
2	S	0.32	0/1176	0.64	0/1589
2	T	0.34	0/1166	0.63	0/1570
2	U	0.33	0/1178	0.69	0/1589
2	V	0.30	0/1158	0.62	3/1558 (0.2%)
2	W	0.34	0/1145	0.70	1/1546 (0.1%)
2	X	0.35	0/1130	0.64	0/1523
All	All	0.32	0/32286	0.62	10/43760 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	160	MET	CA-CB-CG	8.81	128.28	113.30
2	W	75	ILE	CG1-CB-CG2	-5.90	98.43	111.40
2	V	6	TYR	CB-CG-CD1	5.43	124.26	121.00
2	L	128	LEU	CA-CB-CG	5.34	127.59	115.30
2	J	128	LEU	CA-CB-CG	5.34	127.59	115.30
2	V	55	LEU	CA-CB-CG	5.25	127.39	115.30
1	C	159	LEU	N-CA-C	5.21	125.07	111.00
1	A	37	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	F	160	MET	CA-CB-CG	5.06	121.89	113.30
2	V	6	TYR	CB-CG-CD2	-5.02	117.99	121.00

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	A	1494	0	1464	3	0
1	B	1498	0	1463	4	0
1	C	1481	0	1451	6	0
1	D	1487	0	1453	1	0
1	E	1485	0	1451	4	0
1	F	1495	0	1458	5	0
1	M	1507	0	1470	10	0
1	N	1517	0	1484	14	0
1	O	1476	0	1430	6	0
1	P	1502	0	1474	8	0
1	Q	1481	0	1456	7	0
1	R	1483	0	1450	7	0
2	G	1161	0	1115	8	0
2	H	1145	0	1112	4	0
2	I	1097	0	1062	9	0
2	J	1149	0	1111	4	0
2	K	1157	0	1110	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1089	0	1053	5	0
2	S	1157	0	1095	10	0
2	T	1148	0	1117	3	0
2	U	1159	0	1111	7	0
2	V	1140	0	1111	3	0
2	W	1128	0	1078	8	0
2	X	1113	0	1074	5	0
3	Y	72	0	61	0	0
3	e	72	0	61	0	0
3	f	72	0	61	0	0
3	h	72	0	61	0	0
4	Z	83	0	70	2	0
4	a	83	0	70	0	0
4	i	83	0	70	0	0
4	j	83	0	70	0	0
5	b	61	0	52	0	0
5	c	61	0	52	0	0
5	d	61	0	52	0	0
5	g	61	0	52	0	0
All	All	32413	0	31385	129	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (129) 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)
2:J:10:MET:SD	2:J:86:ARG:NH1	2.64	0.71
1:A:159:LEU:O	1:A:160:MET:HG2	1.96	0.65
2:I:55:LEU:HD22	2:I:93:LYS:HD2	1.81	0.63
1:F:159:LEU:O	1:F:160:MET:HG2	1.99	0.62
1:F:23:ALA:CB	1:F:29:VAL:HG21	2.29	0.61
2:U:5:GLU:HB2	2:U:132:TRP:CZ3	2.36	0.61
1:N:160:MET:HB3	1:N:161:PRO:HA	1.82	0.60
2:X:64:THR:HG21	2:X:113:LEU:HD21	1.82	0.60
2:S:64:THR:HG21	2:S:113:LEU:HD21	1.84	0.59
2:U:64:THR:HG21	2:U:113:LEU:HD21	1.85	0.59
2:G:88:LYS:HE2	2:S:78:VAL:HG21	1.84	0.59
2:I:64:THR:HG21	2:I:113:LEU:HD21	1.84	0.58
2:L:10:MET:SD	2:L:86:ARG:NH1	2.78	0.57
2:W:24:ASP:OD1	2:X:68:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ALA:HB3	1:B:29:VAL:HG21	1.89	0.55
1:M:23:ALA:CB	1:M:29:VAL:HG21	2.37	0.55
2:S:5:GLU:HB2	2:S:132:TRP:CZ3	2.41	0.55
2:W:64:THR:HG21	2:W:113:LEU:HD21	1.88	0.54
1:C:29:VAL:HG12	1:C:91:VAL:CG2	2.37	0.54
1:F:82:ARG:NH2	2:L:32:GLN:OE1	2.41	0.54
2:K:58:GLN:NE2	2:K:84:SER:OG	2.41	0.54
2:J:64:THR:HG21	2:J:113:LEU:HD21	1.90	0.54
2:V:64:THR:HG21	2:V:113:LEU:HD21	1.90	0.54
2:K:64:THR:HG21	2:K:113:LEU:HD21	1.89	0.54
1:P:23:ALA:CB	1:P:29:VAL:HG21	2.37	0.53
2:K:5:GLU:HB2	2:K:132:TRP:CZ3	2.43	0.53
1:F:23:ALA:HB1	1:F:29:VAL:HG21	1.90	0.53
1:P:82:ARG:NH2	2:U:32:GLN:OE1	2.42	0.53
2:G:64:THR:HG21	2:G:113:LEU:HD21	1.91	0.52
1:O:29:VAL:HG12	1:O:91:VAL:CG1	2.39	0.52
1:N:29:VAL:HG12	1:N:91:VAL:CG2	2.38	0.52
1:B:23:ALA:CB	1:B:29:VAL:HG21	2.39	0.51
1:R:23:ALA:CB	1:R:29:VAL:HG21	2.40	0.51
2:I:93:LYS:O	2:I:94:ASP:CB	2.59	0.51
2:T:64:THR:HG21	2:T:113:LEU:HD21	1.91	0.51
1:R:82:ARG:NH2	2:W:32:GLN:OE1	2.45	0.50
1:P:173:GLY:N	1:P:186:ALA:O	2.44	0.50
1:P:23:ALA:HB3	1:P:29:VAL:HG21	1.93	0.50
1:C:159:LEU:C	1:C:160:MET:HG2	2.32	0.49
2:I:146:CYS:O	2:I:147:SER:HB3	2.13	0.49
2:L:64:THR:HG21	2:L:113:LEU:HD21	1.95	0.48
2:S:18:SER:HA	2:S:21:ARG:NH1	2.29	0.48
1:N:159:LEU:O	1:N:160:MET:HB2	2.14	0.48
2:J:58:GLN:OE1	2:J:84:SER:OG	2.32	0.47
2:S:56:LEU:HD23	2:S:60:ILE:HG13	1.96	0.47
1:C:82:ARG:NH2	2:J:32:GLN:OE1	2.47	0.47
2:H:64:THR:HG21	2:H:113:LEU:HD21	1.95	0.47
2:W:71:THR:OG1	2:X:24:ASP:HB3	2.14	0.47
4:Z:1:NAG:O3	4:Z:2:NAG:O5	2.25	0.47
2:G:5:GLU:O	2:G:6:TYR:HB2	2.14	0.47
1:M:23:ALA:HB3	1:M:29:VAL:HG21	1.96	0.47
1:M:76:GLY:HA2	1:N:92:THR:HG21	1.97	0.46
1:O:92:THR:HG21	1:P:76:GLY:HA2	1.98	0.46
2:S:5:GLU:HB2	2:S:132:TRP:CE3	2.51	0.46
2:U:99:ASP:OD1	2:U:100:LYS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:56:LEU:HD23	2:G:60:ILE:HG13	1.97	0.46
1:Q:101:ASN:OD1	1:Q:118:HIS:ND1	2.49	0.46
2:H:43:LEU:HD23	2:H:49:TYR:HA	1.98	0.45
2:X:56:LEU:HD23	2:X:60:ILE:HG13	1.98	0.45
1:E:63:MET:HE3	1:E:66:ASP:HA	1.98	0.45
2:G:56:LEU:CD2	2:G:60:ILE:HD11	2.47	0.45
1:R:23:ALA:HB3	1:R:29:VAL:HG21	1.98	0.45
2:I:56:LEU:HD23	2:I:60:ILE:HG13	1.99	0.45
2:S:56:LEU:CD2	2:S:60:ILE:HD11	2.47	0.45
1:Q:44:ILE:HG21	1:Q:106:MET:HB3	1.98	0.45
2:V:51:LYS:NZ	2:V:94:ASP:OD2	2.39	0.44
2:L:58:GLN:OE1	2:L:84:SER:OG	2.35	0.44
2:W:71:THR:OG1	2:W:72:PRO:HD2	2.17	0.44
2:S:58:GLN:CG	2:S:59:ASP:N	2.81	0.44
2:S:58:GLN:HG3	2:S:59:ASP:N	2.32	0.44
2:W:43:LEU:HD13	2:W:146:CYS:SG	2.57	0.44
1:N:101:ASN:OD1	1:N:118:HIS:ND1	2.50	0.44
1:A:76:GLY:HA2	1:B:92:THR:HG21	1.99	0.44
1:N:78:PHE:CE2	1:N:91:VAL:HG12	2.52	0.44
1:B:101:ASN:OD1	1:B:118:HIS:ND1	2.51	0.44
1:E:173:GLY:N	1:E:187:VAL:HG22	2.33	0.44
1:N:44:ILE:HG21	1:N:106:MET:HB3	1.99	0.44
1:N:159:LEU:O	1:N:160:MET:CB	2.65	0.44
2:G:132:TRP:CZ3	2:G:133:ASN:HB2	2.53	0.43
1:Q:44:ILE:CG2	1:Q:106:MET:HB3	2.47	0.43
1:A:115:LYS:NZ	1:N:110:GLU:OE1	2.51	0.43
1:R:101:ASN:OD1	1:R:118:HIS:ND1	2.52	0.43
2:G:43:LEU:HD13	2:G:146:CYS:SG	2.58	0.43
1:O:91:VAL:HG13	1:O:91:VAL:O	2.19	0.43
1:N:218:TYR:OH	1:R:206:ASP:OD2	2.34	0.43
2:U:56:LEU:HD23	2:U:60:ILE:HG13	1.99	0.43
4:Z:3:BMA:O2	4:Z:7:MAN:H2	2.19	0.43
1:Q:159:LEU:O	1:Q:160:MET:CB	2.66	0.43
1:P:218:TYR:OH	1:Q:206:ASP:OD2	2.36	0.43
2:W:18:SER:HA	2:W:21:ARG:NH1	2.34	0.43
2:H:18:SER:O	2:H:21:ARG:HG2	2.19	0.42
1:M:92:THR:HG21	1:N:76:GLY:HA2	2.00	0.42
1:E:38:VAL:HG12	2:K:29:THR:HA	2.01	0.42
1:E:44:ILE:HG21	1:E:106:MET:HB3	2.02	0.42
2:I:18:SER:HA	2:I:21:ARG:NH1	2.34	0.42
1:F:96:ILE:HD12	1:F:151:PHE:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:56:LEU:CD2	2:I:60:ILE:HD11	2.49	0.42
2:K:60:ILE:O	2:K:64:THR:N	2.49	0.42
2:U:56:LEU:CD2	2:U:60:ILE:HD11	2.50	0.42
1:Q:82:ARG:NH2	2:X:32:GLN:OE1	2.52	0.42
1:M:42:PRO:HG3	1:M:82:ARG:CZ	2.50	0.41
2:G:64:THR:CG2	2:G:113:LEU:HD21	2.50	0.41
2:V:43:LEU:HD13	2:V:146:CYS:SG	2.59	0.41
1:C:91:VAL:HG23	1:C:91:VAL:O	2.21	0.41
1:M:101:ASN:OD1	1:M:118:HIS:ND1	2.53	0.41
2:T:43:LEU:HD23	2:T:49:TYR:HA	2.02	0.41
1:N:82:ARG:NH2	2:T:32:GLN:OE1	2.54	0.41
2:I:81:GLN:O	2:I:85:LEU:HD13	2.21	0.41
2:K:5:GLU:HB2	2:K:132:TRP:CE3	2.55	0.41
2:S:43:LEU:HD13	2:S:146:CYS:SG	2.61	0.41
2:H:64:THR:CG2	2:H:113:LEU:HD21	2.50	0.41
1:M:148:VAL:CG2	1:M:156:VAL:HG22	2.51	0.41
1:P:96:ILE:HD12	1:P:151:PHE:CG	2.56	0.41
1:M:44:ILE:HG21	1:M:106:MET:HB3	2.02	0.41
1:Q:96:ILE:HD12	1:Q:151:PHE:CG	2.56	0.41
2:U:43:LEU:HD13	2:U:146:CYS:SG	2.61	0.41
2:I:43:LEU:HD13	2:I:146:CYS:SG	2.61	0.41
1:M:82:ARG:HG2	1:M:83:SER:N	2.36	0.41
1:N:91:VAL:HG23	1:N:91:VAL:O	2.21	0.41
1:M:218:TYR:OH	1:O:206:ASP:OD2	2.33	0.41
1:R:44:ILE:HG21	1:R:106:MET:HB3	2.03	0.40
2:L:56:LEU:HD23	2:L:60:ILE:HG13	2.02	0.40
1:N:127:LEU:O	1:R:128:SER:HA	2.21	0.40
1:O:76:GLY:HA2	1:P:92:THR:HG21	2.03	0.40
2:W:71:THR:OG1	2:W:72:PRO:CD	2.70	0.40
2:K:56:LEU:HD23	2:K:60:ILE:HG13	2.02	0.40
1:O:160:MET:HB3	1:O:161:PRO:HA	2.03	0.40
1:C:78:PHE:CE2	1:C:91:VAL:HG12	2.56	0.40
1:C:92:THR:HG21	1:D:76:GLY:HA2	2.03	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	184/208 (88%)	177 (96%)	6 (3%)	1 (0%)	29	68
1	B	185/208 (89%)	178 (96%)	7 (4%)	0	100	100
1	C	182/208 (88%)	175 (96%)	6 (3%)	1 (0%)	29	68
1	D	183/208 (88%)	176 (96%)	6 (3%)	1 (0%)	29	68
1	E	183/208 (88%)	176 (96%)	6 (3%)	1 (0%)	29	68
1	F	185/208 (89%)	177 (96%)	7 (4%)	1 (0%)	29	68
1	M	187/208 (90%)	178 (95%)	9 (5%)	0	100	100
1	N	187/208 (90%)	179 (96%)	6 (3%)	2 (1%)	14	52
1	O	182/208 (88%)	176 (97%)	5 (3%)	1 (0%)	29	68
1	P	185/208 (89%)	178 (96%)	6 (3%)	1 (0%)	29	68
1	Q	181/208 (87%)	174 (96%)	6 (3%)	1 (1%)	25	65
1	R	182/208 (88%)	175 (96%)	6 (3%)	1 (0%)	29	68
2	G	143/153 (94%)	139 (97%)	4 (3%)	0	100	100
2	H	140/153 (92%)	136 (97%)	4 (3%)	0	100	100
2	I	133/153 (87%)	130 (98%)	3 (2%)	0	100	100
2	J	140/153 (92%)	136 (97%)	4 (3%)	0	100	100
2	K	141/153 (92%)	139 (99%)	2 (1%)	0	100	100
2	L	131/153 (86%)	128 (98%)	3 (2%)	0	100	100
2	S	142/153 (93%)	138 (97%)	4 (3%)	0	100	100
2	T	140/153 (92%)	136 (97%)	4 (3%)	0	100	100
2	U	142/153 (93%)	138 (97%)	4 (3%)	0	100	100
2	V	137/153 (90%)	133 (97%)	4 (3%)	0	100	100
2	W	138/153 (90%)	134 (97%)	4 (3%)	0	100	100
2	X	135/153 (88%)	130 (96%)	5 (4%)	0	100	100
All	All	3868/4332 (89%)	3736 (97%)	121 (3%)	11 (0%)	41	76

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	160	MET
1	A	41	GLY
1	C	41	GLY
1	D	41	GLY
1	E	41	GLY
1	F	41	GLY
1	N	41	GLY
1	O	41	GLY
1	P	41	GLY
1	Q	41	GLY
1	R	41	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	A	166/183 (91%)	166 (100%)	0	100 100
1	B	167/183 (91%)	167 (100%)	0	100 100
1	C	165/183 (90%)	165 (100%)	0	100 100
1	D	166/183 (91%)	166 (100%)	0	100 100
1	E	165/183 (90%)	165 (100%)	0	100 100
1	F	165/183 (90%)	165 (100%)	0	100 100
1	M	166/183 (91%)	166 (100%)	0	100 100
1	N	169/183 (92%)	168 (99%)	1 (1%)	86 92
1	O	164/183 (90%)	164 (100%)	0	100 100
1	P	168/183 (92%)	168 (100%)	0	100 100
1	Q	166/183 (91%)	166 (100%)	0	100 100
1	R	166/183 (91%)	166 (100%)	0	100 100
2	G	133/145 (92%)	132 (99%)	1 (1%)	81 89
2	H	131/145 (90%)	130 (99%)	1 (1%)	81 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	127/145 (88%)	125 (98%)	2 (2%)	62	79
2	J	132/145 (91%)	131 (99%)	1 (1%)	81	89
2	K	133/145 (92%)	132 (99%)	1 (1%)	81	89
2	L	125/145 (86%)	124 (99%)	1 (1%)	81	89
2	S	132/145 (91%)	131 (99%)	1 (1%)	81	89
2	T	132/145 (91%)	131 (99%)	1 (1%)	81	89
2	U	133/145 (92%)	131 (98%)	2 (2%)	65	80
2	V	131/145 (90%)	130 (99%)	1 (1%)	81	89
2	W	128/145 (88%)	126 (98%)	2 (2%)	62	79
2	X	128/145 (88%)	127 (99%)	1 (1%)	81	89
All	All	3558/3936 (90%)	3542 (100%)	16 (0%)	91	94

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	30	SER
2	H	30	SER
2	I	30	SER
2	I	85	LEU
2	J	30	SER
2	K	30	SER
2	L	30	SER
1	N	172	ASN
2	S	30	SER
2	T	30	SER
2	U	30	SER
2	U	147	SER
2	V	30	SER
2	W	30	SER
2	W	75	ILE
2	X	30	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
2	G	9	HIS

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Mol	Chain	Res	Type
2	K	58	GLN
1	M	81	HIS
2	V	42	GLN
2	W	70	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

72 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	Y	1	1,3	14,14,15	0.52	0	17,19,21	1.04	1 (5%)
3	NAG	Y	2	3	14,14,15	0.55	0	17,19,21	0.63	0
3	BMA	Y	3	3	11,11,12	0.68	0	15,15,17	0.91	0
3	MAN	Y	4	3	11,11,12	0.57	0	15,15,17	0.95	1 (6%)
3	MAN	Y	5	3	11,11,12	0.61	0	15,15,17	1.03	1 (6%)
3	MAN	Y	6	3	11,11,12	0.61	0	15,15,17	0.75	1 (6%)
4	NAG	Z	1	1,4	14,14,15	0.58	0	17,19,21	1.29	3 (17%)
4	NAG	Z	2	4	14,14,15	0.54	0	17,19,21	0.89	0
4	BMA	Z	3	4	11,11,12	0.62	0	15,15,17	2.15	2 (13%)
4	MAN	Z	4	4	11,11,12	0.54	0	15,15,17	1.64	2 (13%)
4	MAN	Z	5	4	11,11,12	0.60	0	15,15,17	0.67	0
4	MAN	Z	6	4	11,11,12	0.60	0	15,15,17	1.00	1 (6%)
4	MAN	Z	7	4	11,11,12	0.66	0	15,15,17	1.56	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	a	1	1,4	14,14,15	0.52	0	17,19,21	1.54	2 (11%)
4	NAG	a	2	4	14,14,15	0.56	0	17,19,21	0.93	0
4	BMA	a	3	4	11,11,12	0.57	0	15,15,17	1.82	3 (20%)
4	MAN	a	4	4	11,11,12	0.60	0	15,15,17	1.39	2 (13%)
4	MAN	a	5	4	11,11,12	0.61	0	15,15,17	0.83	0
4	MAN	a	6	4	11,11,12	0.56	0	15,15,17	0.78	0
4	MAN	a	7	4	11,11,12	0.65	0	15,15,17	0.88	1 (6%)
5	NAG	b	1	1,5	14,14,15	0.58	0	17,19,21	1.75	4 (23%)
5	NAG	b	2	5	14,14,15	0.59	0	17,19,21	0.98	1 (5%)
5	BMA	b	3	5	11,11,12	0.59	0	15,15,17	1.59	3 (20%)
5	MAN	b	4	5	11,11,12	0.64	0	15,15,17	0.87	1 (6%)
5	MAN	b	5	5	11,11,12	0.53	0	15,15,17	0.85	1 (6%)
5	NAG	c	1	1,5	14,14,15	0.65	0	17,19,21	1.05	1 (5%)
5	NAG	c	2	5	14,14,15	0.59	0	17,19,21	0.97	0
5	BMA	c	3	5	11,11,12	0.71	0	15,15,17	1.79	3 (20%)
5	MAN	c	4	5	11,11,12	0.50	0	15,15,17	1.23	2 (13%)
5	MAN	c	5	5	11,11,12	0.59	0	15,15,17	0.97	1 (6%)
5	NAG	d	1	1,5	14,14,15	0.56	0	17,19,21	1.46	3 (17%)
5	NAG	d	2	5	14,14,15	0.54	0	17,19,21	0.88	1 (5%)
5	BMA	d	3	5	11,11,12	0.78	0	15,15,17	1.49	1 (6%)
5	MAN	d	4	5	11,11,12	0.54	0	15,15,17	1.06	2 (13%)
5	MAN	d	5	5	11,11,12	0.59	0	15,15,17	0.86	0
3	NAG	e	1	1,3	14,14,15	0.55	0	17,19,21	1.12	1 (5%)
3	NAG	e	2	3	14,14,15	0.54	0	17,19,21	0.67	0
3	BMA	e	3	3	11,11,12	0.71	0	15,15,17	0.91	0
3	MAN	e	4	3	11,11,12	0.55	0	15,15,17	1.32	2 (13%)
3	MAN	e	5	3	11,11,12	0.69	0	15,15,17	0.72	0
3	MAN	e	6	3	11,11,12	0.60	0	15,15,17	0.87	0
3	NAG	f	1	1,3	14,14,15	0.59	0	17,19,21	1.41	3 (17%)
3	NAG	f	2	3	14,14,15	0.58	0	17,19,21	0.75	0
3	BMA	f	3	3	11,11,12	0.72	0	15,15,17	1.60	3 (20%)
3	MAN	f	4	3	11,11,12	0.50	0	15,15,17	1.46	2 (13%)
3	MAN	f	5	3	11,11,12	0.52	0	15,15,17	1.26	1 (6%)
3	MAN	f	6	3	11,11,12	0.50	0	15,15,17	1.08	2 (13%)
5	NAG	g	1	1,5	14,14,15	0.61	0	17,19,21	0.98	1 (5%)
5	NAG	g	2	5	14,14,15	0.55	0	17,19,21	0.78	0
5	BMA	g	3	5	11,11,12	0.59	0	15,15,17	1.65	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	g	4	5	11,11,12	0.58	0	15,15,17	0.93	1 (6%)
5	MAN	g	5	5	11,11,12	0.56	0	15,15,17	1.00	1 (6%)
3	NAG	h	1	1,3	14,14,15	0.55	0	17,19,21	1.16	2 (11%)
3	NAG	h	2	3	14,14,15	0.58	0	17,19,21	1.10	1 (5%)
3	BMA	h	3	3	11,11,12	0.82	0	15,15,17	1.20	1 (6%)
3	MAN	h	4	3	11,11,12	0.62	0	15,15,17	0.80	1 (6%)
3	MAN	h	5	3	11,11,12	0.66	0	15,15,17	0.70	0
3	MAN	h	6	3	11,11,12	0.66	0	15,15,17	1.00	1 (6%)
4	NAG	i	1	1,4	14,14,15	0.54	0	17,19,21	1.28	3 (17%)
4	NAG	i	2	4	14,14,15	0.52	0	17,19,21	0.68	0
4	BMA	i	3	4	11,11,12	0.77	0	15,15,17	1.32	3 (20%)
4	MAN	i	4	4	11,11,12	0.60	0	15,15,17	1.64	3 (20%)
4	MAN	i	5	4	11,11,12	0.60	0	15,15,17	0.91	1 (6%)
4	MAN	i	6	4	11,11,12	0.51	0	15,15,17	1.28	2 (13%)
4	MAN	i	7	4	11,11,12	0.61	0	15,15,17	1.13	1 (6%)
4	NAG	j	1	1,4	14,14,15	0.51	0	17,19,21	1.32	2 (11%)
4	NAG	j	2	4	14,14,15	0.58	0	17,19,21	0.86	1 (5%)
4	BMA	j	3	4	11,11,12	0.70	0	15,15,17	1.78	5 (33%)
4	MAN	j	4	4	11,11,12	0.63	0	15,15,17	1.10	1 (6%)
4	MAN	j	5	4	11,11,12	0.59	0	15,15,17	1.03	1 (6%)
4	MAN	j	6	4	11,11,12	0.65	0	15,15,17	0.90	1 (6%)
4	MAN	j	7	4	11,11,12	0.48	0	15,15,17	2.05	3 (20%)

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	Y	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Y	3	3	-	1/2/19/22	0/1/1/1
3	MAN	Y	4	3	-	2/2/19/22	0/1/1/1
3	MAN	Y	5	3	-	2/2/19/22	0/1/1/1
3	MAN	Y	6	3	-	0/2/19/22	0/1/1/1
4	NAG	Z	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	Z	3	4	-	1/2/19/22	0/1/1/1
4	MAN	Z	4	4	-	2/2/19/22	0/1/1/1
4	MAN	Z	5	4	-	2/2/19/22	0/1/1/1
4	MAN	Z	6	4	-	0/2/19/22	0/1/1/1
4	MAN	Z	7	4	-	0/2/19/22	0/1/1/1
4	NAG	a	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	a	2	4	-	3/6/23/26	0/1/1/1
4	BMA	a	3	4	-	2/2/19/22	0/1/1/1
4	MAN	a	4	4	-	0/2/19/22	0/1/1/1
4	MAN	a	5	4	-	0/2/19/22	0/1/1/1
4	MAN	a	6	4	-	0/2/19/22	0/1/1/1
4	MAN	a	7	4	-	2/2/19/22	0/1/1/1
5	NAG	b	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	b	2	5	-	2/6/23/26	0/1/1/1
5	BMA	b	3	5	-	0/2/19/22	0/1/1/1
5	MAN	b	4	5	-	2/2/19/22	0/1/1/1
5	MAN	b	5	5	-	0/2/19/22	0/1/1/1
5	NAG	c	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	6/6/23/26	0/1/1/1
5	BMA	c	3	5	-	2/2/19/22	0/1/1/1
5	MAN	c	4	5	-	0/2/19/22	0/1/1/1
5	MAN	c	5	5	-	2/2/19/22	0/1/1/1
5	NAG	d	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	0/6/23/26	0/1/1/1
5	BMA	d	3	5	-	1/2/19/22	0/1/1/1
5	MAN	d	4	5	-	1/2/19/22	0/1/1/1
5	MAN	d	5	5	-	0/2/19/22	0/1/1/1
3	NAG	e	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	e	2	3	-	0/6/23/26	0/1/1/1
3	BMA	e	3	3	-	1/2/19/22	0/1/1/1
3	MAN	e	4	3	-	1/2/19/22	0/1/1/1
3	MAN	e	5	3	-	2/2/19/22	0/1/1/1
3	MAN	e	6	3	-	0/2/19/22	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
3	BMA	f	3	3	-	1/2/19/22	0/1/1/1
3	MAN	f	4	3	-	1/2/19/22	0/1/1/1
3	MAN	f	5	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	f	6	3	-	0/2/19/22	0/1/1/1
5	NAG	g	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	g	2	5	-	2/6/23/26	0/1/1/1
5	BMA	g	3	5	-	2/2/19/22	0/1/1/1
5	MAN	g	4	5	-	1/2/19/22	0/1/1/1
5	MAN	g	5	5	-	2/2/19/22	0/1/1/1
3	NAG	h	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	h	2	3	-	2/6/23/26	0/1/1/1
3	BMA	h	3	3	-	2/2/19/22	0/1/1/1
3	MAN	h	4	3	-	0/2/19/22	0/1/1/1
3	MAN	h	5	3	-	0/2/19/22	0/1/1/1
3	MAN	h	6	3	-	2/2/19/22	0/1/1/1
4	NAG	i	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	i	2	4	-	1/6/23/26	0/1/1/1
4	BMA	i	3	4	-	2/2/19/22	0/1/1/1
4	MAN	i	4	4	-	1/2/19/22	0/1/1/1
4	MAN	i	5	4	-	0/2/19/22	0/1/1/1
4	MAN	i	6	4	-	1/2/19/22	0/1/1/1
4	MAN	i	7	4	-	0/2/19/22	0/1/1/1
4	NAG	j	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	j	2	4	-	2/6/23/26	0/1/1/1
4	BMA	j	3	4	-	2/2/19/22	0/1/1/1
4	MAN	j	4	4	-	2/2/19/22	0/1/1/1
4	MAN	j	5	4	-	0/2/19/22	0/1/1/1
4	MAN	j	6	4	-	2/2/19/22	0/1/1/1
4	MAN	j	7	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Z	3	BMA	O3-C3-C2	6.91	123.23	109.99
4	j	7	MAN	C1-O5-C5	6.38	120.84	112.19
5	d	3	BMA	O2-C2-C1	4.69	118.76	109.15
4	a	3	BMA	C1-O5-C5	4.66	118.50	112.19
4	Z	4	MAN	C1-C2-C3	4.44	115.12	109.67
5	c	3	BMA	O3-C3-C2	4.38	118.39	109.99
5	b	3	BMA	C1-C2-C3	4.34	115.00	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	f	4	MAN	C1-O5-C5	4.30	118.02	112.19
4	a	3	BMA	C1-C2-C3	4.23	114.86	109.67
5	b	1	NAG	O5-C1-C2	-4.07	104.86	111.29
4	Z	7	MAN	O5-C1-C2	-3.89	104.77	110.77
4	Z	4	MAN	C1-O5-C5	3.87	117.44	112.19
5	g	3	BMA	C1-C2-C3	3.84	114.39	109.67
3	h	3	BMA	O2-C2-C1	3.77	116.87	109.15
4	a	1	NAG	O5-C1-C2	-3.69	105.46	111.29
4	j	3	BMA	C1-C2-C3	3.64	114.14	109.67
3	e	4	MAN	C1-C2-C3	3.60	114.09	109.67
3	f	5	MAN	C1-O5-C5	3.56	117.01	112.19
4	a	1	NAG	C1-O5-C5	3.54	116.99	112.19
4	i	6	MAN	C1-O5-C5	3.35	116.74	112.19
5	c	4	MAN	C1-O5-C5	3.34	116.71	112.19
5	d	1	NAG	C1-O5-C5	3.31	116.68	112.19
5	b	1	NAG	C1-O5-C5	3.31	116.67	112.19
4	a	4	MAN	O5-C1-C2	-3.31	105.67	110.77
4	i	7	MAN	C1-C2-C3	3.24	113.65	109.67
3	e	1	NAG	O5-C5-C6	3.19	112.20	107.20
4	j	7	MAN	C1-C2-C3	3.18	113.57	109.67
3	f	3	BMA	C1-O5-C5	3.14	116.45	112.19
5	c	3	BMA	C1-O5-C5	3.10	116.39	112.19
4	j	1	NAG	O5-C1-C2	-3.09	106.41	111.29
3	h	6	MAN	C1-C2-C3	3.05	113.42	109.67
4	i	4	MAN	C1-O5-C5	3.05	116.33	112.19
3	h	2	NAG	C1-O5-C5	3.02	116.28	112.19
4	j	3	BMA	O5-C5-C6	3.01	111.92	107.20
4	i	4	MAN	O3-C3-C2	2.97	115.67	109.99
5	d	4	MAN	C1-O5-C5	2.91	116.13	112.19
3	f	3	BMA	O3-C3-C4	2.90	117.06	110.35
4	Z	3	BMA	C1-O5-C5	2.89	116.11	112.19
5	g	5	MAN	C1-O5-C5	2.89	116.11	112.19
5	c	3	BMA	C1-C2-C3	2.86	113.18	109.67
5	c	1	NAG	O5-C1-C2	-2.85	106.78	111.29
4	j	5	MAN	C1-C2-C3	2.84	113.15	109.67
3	f	3	BMA	O5-C5-C6	-2.83	102.77	107.20
3	f	4	MAN	C1-C2-C3	2.82	113.13	109.67
5	b	3	BMA	C1-O5-C5	2.76	115.93	112.19
4	j	4	MAN	O3-C3-C2	2.76	115.27	109.99
3	Y	1	NAG	C1-O5-C5	2.75	115.92	112.19
5	g	3	BMA	O3-C3-C4	2.75	116.70	110.35
3	e	4	MAN	C1-O5-C5	2.70	115.85	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	a	4	MAN	O3-C3-C4	2.70	116.59	110.35
5	b	1	NAG	C1-C2-N2	2.68	115.06	110.49
5	d	1	NAG	C6-C5-C4	-2.66	106.77	113.00
5	b	5	MAN	O5-C5-C6	2.64	111.34	107.20
3	f	1	NAG	O5-C1-C2	-2.63	107.14	111.29
4	j	3	BMA	C3-C4-C5	-2.61	105.58	110.24
5	g	4	MAN	C1-O5-C5	2.59	115.70	112.19
4	Z	7	MAN	C1-C2-C3	2.58	112.84	109.67
4	i	1	NAG	O5-C1-C2	-2.57	107.23	111.29
4	i	3	BMA	C1-O5-C5	-2.56	108.72	112.19
5	g	3	BMA	O3-C3-C2	-2.56	105.09	109.99
4	i	3	BMA	O5-C1-C2	-2.56	106.82	110.77
4	Z	1	NAG	C3-C4-C5	-2.55	105.69	110.24
3	Y	5	MAN	O5-C5-C6	2.52	111.15	107.20
4	Z	6	MAN	O5-C5-C6	2.50	111.12	107.20
4	i	5	MAN	C1-C2-C3	2.47	112.71	109.67
4	j	1	NAG	O5-C5-C6	2.45	111.05	107.20
4	i	1	NAG	C6-C5-C4	-2.45	107.26	113.00
4	Z	1	NAG	O5-C1-C2	-2.40	107.50	111.29
4	a	7	MAN	C1-C2-C3	2.40	112.61	109.67
5	c	5	MAN	O5-C5-C6	2.38	110.94	107.20
4	i	1	NAG	C4-C3-C2	2.35	114.45	111.02
5	d	1	NAG	O5-C1-C2	-2.34	107.59	111.29
3	f	1	NAG	C1-O5-C5	2.34	115.36	112.19
3	h	1	NAG	O5-C1-C2	-2.32	107.63	111.29
5	g	1	NAG	C1-O5-C5	2.30	115.31	112.19
4	i	6	MAN	C2-C3-C4	-2.29	106.92	110.89
4	j	6	MAN	O5-C5-C6	2.28	110.78	107.20
5	b	3	BMA	O5-C5-C6	2.27	110.76	107.20
4	i	4	MAN	O5-C5-C6	2.24	110.71	107.20
5	b	1	NAG	C6-C5-C4	-2.24	107.77	113.00
3	h	4	MAN	O5-C5-C6	2.23	110.70	107.20
4	j	3	BMA	O4-C4-C3	2.23	115.50	110.35
4	j	2	NAG	O5-C5-C6	2.23	110.69	107.20
3	f	1	NAG	C6-C5-C4	-2.23	107.79	113.00
5	d	2	NAG	C1-O5-C5	2.22	115.20	112.19
4	j	7	MAN	C6-C5-C4	-2.21	107.83	113.00
3	f	6	MAN	O5-C5-C6	2.21	110.66	107.20
3	f	6	MAN	O5-C1-C2	-2.16	107.44	110.77
5	b	2	NAG	C1-O5-C5	2.12	115.06	112.19
5	d	4	MAN	C1-C2-C3	2.11	112.26	109.67
4	i	3	BMA	O5-C5-C6	2.09	110.48	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	b	4	MAN	C1-C2-C3	2.09	112.23	109.67
3	Y	6	MAN	O5-C1-C2	-2.08	107.56	110.77
4	j	3	BMA	C2-C3-C4	-2.07	107.32	110.89
4	a	3	BMA	C6-C5-C4	-2.07	108.16	113.00
4	Z	7	MAN	C1-O5-C5	-2.05	109.42	112.19
3	Y	4	MAN	O5-C1-C2	-2.04	107.62	110.77
5	c	4	MAN	C6-C5-C4	-2.03	108.24	113.00
3	h	1	NAG	O5-C5-C6	2.03	110.39	107.20
4	Z	1	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	i	1	NAG	C8-C7-N2-C2
4	i	1	NAG	O7-C7-N2-C2
4	a	2	NAG	C3-C2-N2-C7
5	c	2	NAG	C8-C7-N2-C2
5	c	2	NAG	O7-C7-N2-C2
4	j	1	NAG	C1-C2-N2-C7
5	c	3	BMA	C4-C5-C6-O6
4	j	3	BMA	C4-C5-C6-O6
4	Z	4	MAN	O5-C5-C6-O6
5	c	3	BMA	O5-C5-C6-O6
4	j	3	BMA	O5-C5-C6-O6
4	i	1	NAG	C1-C2-N2-C7
4	a	7	MAN	O5-C5-C6-O6
4	a	3	BMA	O5-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	f	1	NAG	O5-C5-C6-O6
4	a	7	MAN	C4-C5-C6-O6
5	g	2	NAG	C4-C5-C6-O6
5	g	2	NAG	O5-C5-C6-O6
4	j	7	MAN	O5-C5-C6-O6
4	Z	5	MAN	O5-C5-C6-O6
3	f	5	MAN	C4-C5-C6-O6
4	Z	4	MAN	C4-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
3	h	3	BMA	O5-C5-C6-O6
3	h	3	BMA	C4-C5-C6-O6
3	f	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	Y	4	MAN	O5-C5-C6-O6
4	a	3	BMA	C4-C5-C6-O6
3	e	1	NAG	C1-C2-N2-C7
5	b	1	NAG	C1-C2-N2-C7
5	c	2	NAG	C1-C2-N2-C7
5	b	4	MAN	C4-C5-C6-O6
3	Y	4	MAN	C4-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
3	f	2	NAG	C4-C5-C6-O6
5	c	5	MAN	O5-C5-C6-O6
3	h	6	MAN	C4-C5-C6-O6
4	j	2	NAG	O5-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
4	Z	5	MAN	C4-C5-C6-O6
5	b	4	MAN	O5-C5-C6-O6
4	j	1	NAG	O5-C5-C6-O6
5	c	5	MAN	C4-C5-C6-O6
3	h	1	NAG	C8-C7-N2-C2
3	Y	1	NAG	C4-C5-C6-O6
5	g	4	MAN	O5-C5-C6-O6
5	g	1	NAG	C4-C5-C6-O6
3	h	6	MAN	O5-C5-C6-O6
4	i	2	NAG	O5-C5-C6-O6
3	h	1	NAG	O5-C5-C6-O6
3	h	2	NAG	C4-C5-C6-O6
3	f	1	NAG	C4-C5-C6-O6
5	g	5	MAN	C4-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
3	h	1	NAG	O7-C7-N2-C2
3	f	3	BMA	O5-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
4	j	4	MAN	C4-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
3	e	4	MAN	O5-C5-C6-O6
3	Y	3	BMA	O5-C5-C6-O6
5	g	1	NAG	O5-C5-C6-O6
4	j	6	MAN	C4-C5-C6-O6
4	Z	3	BMA	O5-C5-C6-O6
5	d	3	BMA	O5-C5-C6-O6
3	e	3	BMA	O5-C5-C6-O6
4	i	3	BMA	O5-C5-C6-O6
4	Z	1	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	c	2	NAG	C3-C2-N2-C7
5	c	2	NAG	C4-C5-C6-O6
4	j	6	MAN	O5-C5-C6-O6
5	g	5	MAN	O5-C5-C6-O6
3	e	5	MAN	C4-C5-C6-O6
3	Y	1	NAG	O5-C5-C6-O6
4	j	7	MAN	C4-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
4	j	4	MAN	O5-C5-C6-O6
3	e	5	MAN	O5-C5-C6-O6
3	Y	5	MAN	O5-C5-C6-O6
5	b	2	NAG	C4-C5-C6-O6
4	i	6	MAN	C4-C5-C6-O6
4	j	2	NAG	C4-C5-C6-O6
3	Y	5	MAN	C4-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
5	g	3	BMA	C4-C5-C6-O6
5	g	3	BMA	O5-C5-C6-O6
5	c	1	NAG	C3-C2-N2-C7
3	f	4	MAN	C4-C5-C6-O6
3	e	1	NAG	C8-C7-N2-C2
3	e	1	NAG	O7-C7-N2-C2
4	i	4	MAN	O5-C5-C6-O6
5	d	4	MAN	C4-C5-C6-O6
4	i	3	BMA	C4-C5-C6-O6

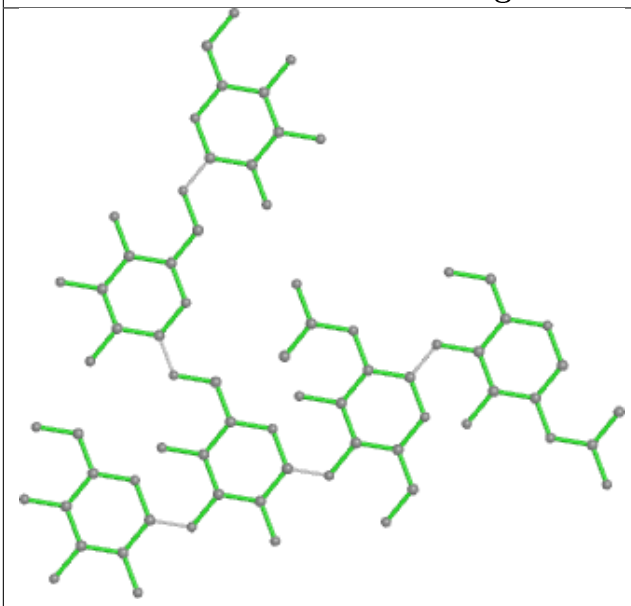
There are no ring outliers.

4 monomers are involved in 2 short contacts:

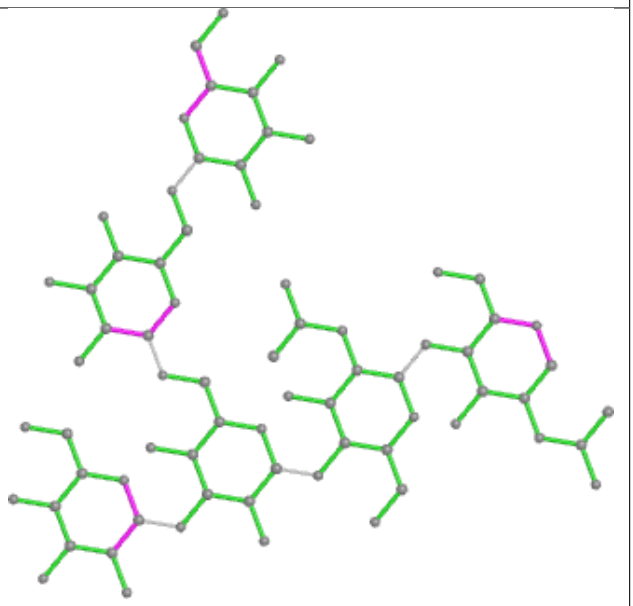
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Z	1	NAG	1	0
4	Z	2	NAG	1	0
4	Z	3	BMA	1	0
4	Z	7	MAN	1	0

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

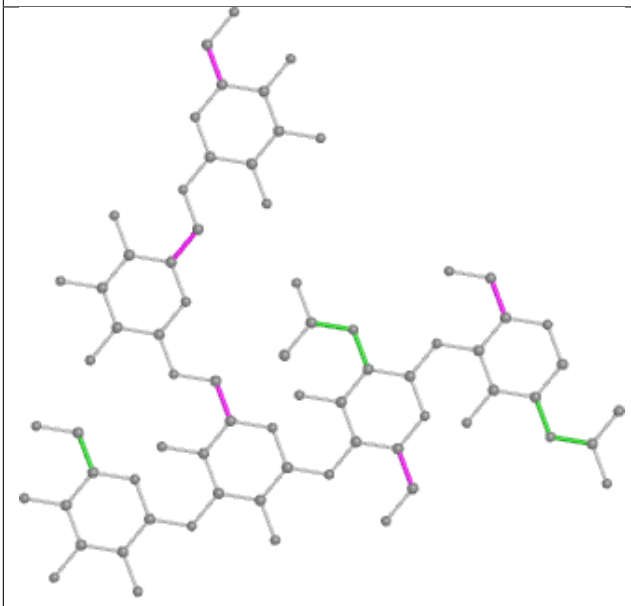
Oligosaccharide Chain Y



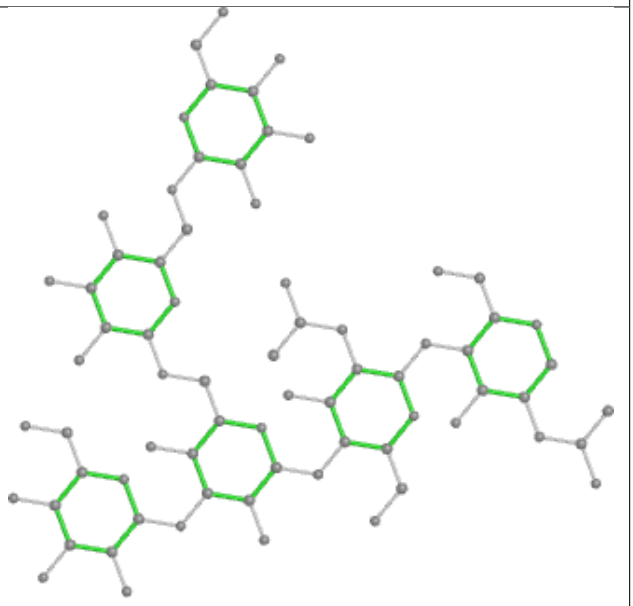
Bond lengths



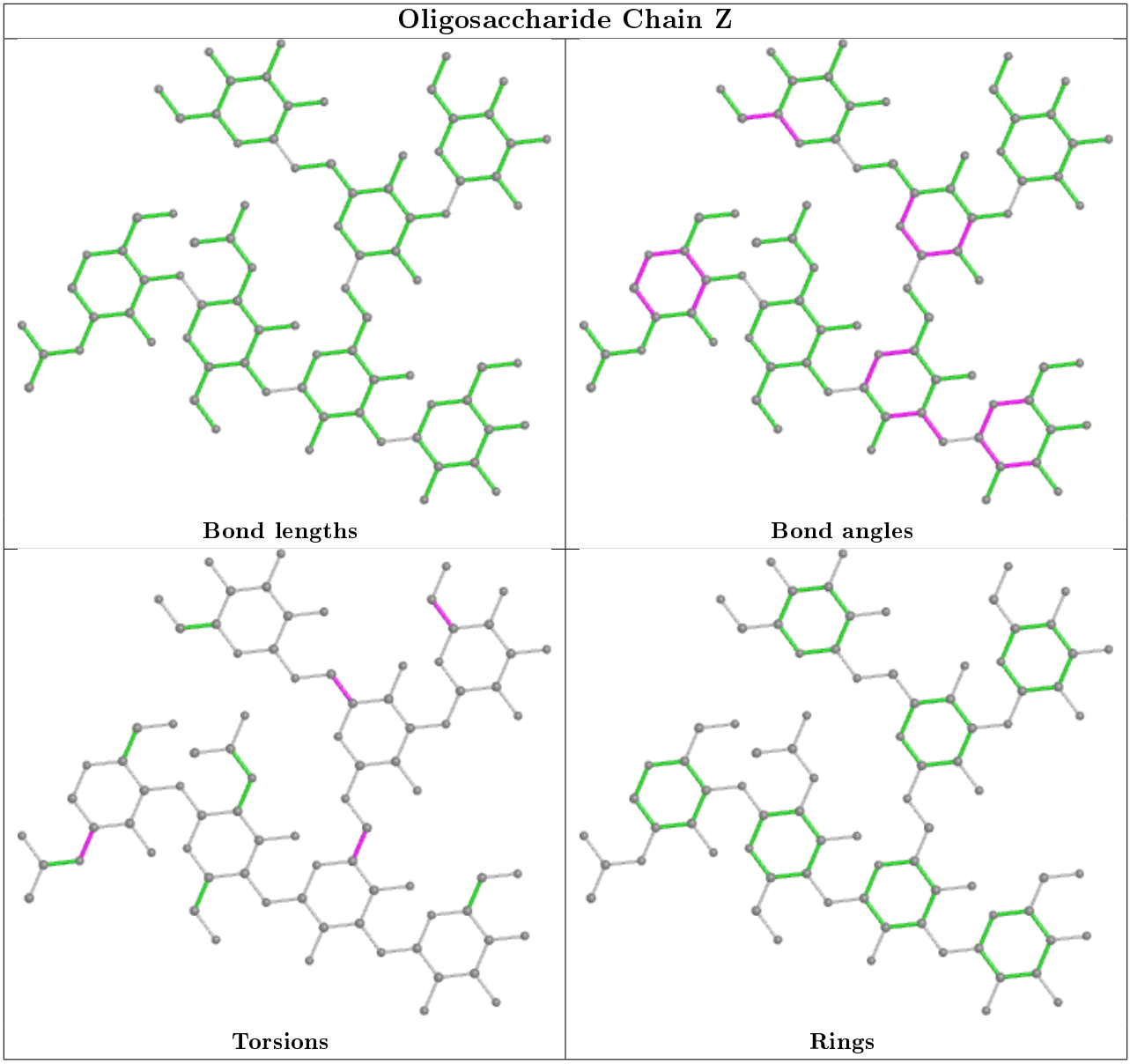
Bond angles



Torsions



Rings



5.6 Ligand geometry

There are no ligands in this entry.

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	A	188/208 (90%)	0.26	1 (0%) 91 85	143, 190, 239, 281	0
1	B	189/208 (90%)	0.34	5 (2%) 56 46	146, 194, 242, 283	0
1	C	186/208 (89%)	0.55	19 (10%) 6 7	157, 209, 248, 289	0
1	D	187/208 (89%)	0.19	4 (2%) 63 54	150, 202, 238, 288	0
1	E	187/208 (89%)	0.62	24 (12%) 3 4	167, 212, 249, 290	0
1	F	189/208 (90%)	0.21	6 (3%) 47 37	145, 205, 246, 291	0
1	M	191/208 (91%)	0.19	1 (0%) 91 85	143, 193, 248, 317	0
1	N	191/208 (91%)	0.32	3 (1%) 72 62	142, 189, 242, 289	0
1	O	186/208 (89%)	0.11	0 100 100	132, 196, 237, 280	0
1	P	189/208 (90%)	0.23	3 (1%) 72 62	153, 193, 245, 281	0
1	Q	185/208 (88%)	0.28	5 (2%) 54 45	146, 199, 240, 280	0
1	R	186/208 (89%)	0.09	1 (0%) 91 85	135, 192, 238, 285	0
2	G	145/153 (94%)	0.36	1 (0%) 87 82	140, 215, 266, 338	0
2	H	142/153 (92%)	0.12	1 (0%) 87 82	155, 230, 283, 323	0
2	I	137/153 (89%)	0.50	10 (7%) 15 12	178, 246, 290, 316	0
2	J	142/153 (92%)	0.26	7 (4%) 29 25	184, 250, 298, 334	0
2	K	143/153 (93%)	0.28	17 (11%) 4 5	179, 248, 296, 336	0
2	L	135/153 (88%)	0.91	26 (19%) 1 1	187, 248, 301, 350	0
2	S	144/153 (94%)	0.16	0 100 100	161, 225, 278, 327	0
2	T	142/153 (92%)	0.11	4 (2%) 53 43	164, 240, 292, 331	0
2	U	144/153 (94%)	-0.02	0 100 100	176, 243, 299, 325	0
2	V	141/153 (92%)	0.24	8 (5%) 23 20	166, 237, 280, 324	0
2	W	142/153 (92%)	0.20	2 (1%) 75 66	169, 235, 288, 321	0
2	X	139/153 (90%)	0.15	2 (1%) 75 66	159, 228, 282, 314	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	3950/4332 (91%)	0.28	150 (3%) 40 32	132, 210, 279, 350	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	190	SER	6.0
2	L	7	CYS	5.0
1	C	189	LEU	4.7
2	L	53	ALA	4.6
2	L	44	LYS	4.6
2	I	86	ARG	4.3
2	L	70	ASN	4.3
1	C	142	LEU	4.2
1	C	199	VAL	4.2
2	K	92	THR	4.1
2	K	135	PHE	3.9
2	L	98	HIS	3.9
2	L	52	LYS	3.9
2	V	98	HIS	3.9
2	K	96	GLU	3.9
2	I	135	PHE	3.8
2	K	36	GLU	3.8
1	E	78	PHE	3.6
1	E	156	VAL	3.6
1	B	129	VAL	3.6
1	E	199	VAL	3.5
1	C	156	VAL	3.4
1	F	78	PHE	3.4
2	K	98	HIS	3.4
1	E	41	GLY	3.4
1	C	191	LEU	3.3
1	B	214	TYR	3.3
2	K	136	SER	3.3
1	C	157	GLN	3.3
1	D	123	LYS	3.3
1	E	155	HIS	3.2
2	V	36	GLU	3.2
2	L	46	PRO	3.2
2	L	45	ASP	3.1
2	J	97	GLU	3.1
1	Q	156	VAL	3.0
1	F	210	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	L	36	GLU	3.0
2	X	135	PHE	3.0
1	N	204	LYS	2.9
1	E	154	PRO	2.9
2	L	49	TYR	2.8
1	C	214	TYR	2.8
2	L	86	ARG	2.8
2	L	144	ALA	2.8
1	B	203	GLY	2.8
1	E	158	TRP	2.8
1	C	159	LEU	2.8
1	Q	204	LYS	2.8
2	L	54	PHE	2.8
2	L	9	HIS	2.7
1	Q	159	LEU	2.7
2	T	11	ILE	2.7
1	C	143	THR	2.7
2	W	8	SER	2.7
1	E	200	THR	2.7
2	I	54	PHE	2.7
2	I	11	ILE	2.7
2	J	11	ILE	2.7
1	E	121	VAL	2.7
1	C	151	PHE	2.6
1	E	40	LEU	2.6
1	E	211	HIS	2.6
2	T	91	PHE	2.6
1	C	62	ARG	2.6
1	E	203	GLY	2.6
1	E	191	LEU	2.6
1	Q	200	THR	2.6
2	L	47	VAL	2.6
2	K	134	ILE	2.6
1	R	35	TRP	2.5
2	I	121	PHE	2.5
2	K	133	ASN	2.5
1	P	214	TYR	2.5
1	N	156	VAL	2.5
1	E	204	LYS	2.5
1	N	62	ARG	2.5
2	L	51	LYS	2.5
2	K	38	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	J	67	PHE	2.5
2	V	38	VAL	2.4
2	I	36	GLU	2.4
1	C	154	PRO	2.4
2	K	11	ILE	2.4
1	E	214	TYR	2.4
1	F	79	ASP	2.4
1	B	133	ARG	2.4
2	J	132	TRP	2.4
1	E	159	LEU	2.4
2	K	41	GLU	2.4
2	L	141	ASN	2.4
1	D	122	VAL	2.4
2	I	124	THR	2.4
2	K	94	ASP	2.4
2	L	11	ILE	2.3
1	C	211	HIS	2.3
1	E	189	LEU	2.3
2	L	10	MET	2.3
1	F	211	HIS	2.3
1	C	158	TRP	2.3
2	I	44	LYS	2.3
2	V	143	PHE	2.3
2	X	90	CYS	2.3
1	B	213	VAL	2.3
2	L	138	ASN	2.3
1	E	102	TYR	2.3
2	J	28	GLU	2.3
2	K	97	GLU	2.3
2	H	135	PHE	2.3
2	L	140	ASN	2.3
1	P	219	LEU	2.3
2	J	133	ASN	2.3
2	G	96	GLU	2.3
2	L	142	SER	2.3
1	F	214	TYR	2.3
1	D	41	GLY	2.3
1	F	35	TRP	2.3
1	E	157	GLN	2.3
1	M	63	MET	2.2
1	E	79	ASP	2.2
2	K	28	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	78	PHE	2.2
2	I	132	TRP	2.2
2	V	121	PHE	2.2
2	K	93	LYS	2.2
2	W	86	ARG	2.2
1	C	200	THR	2.2
2	K	52	LYS	2.2
2	K	121	PHE	2.2
2	V	43	LEU	2.2
1	E	190	SER	2.2
2	J	38	VAL	2.2
1	A	148	VAL	2.1
2	L	121	PHE	2.1
2	I	90	CYS	2.1
2	V	10	MET	2.1
2	L	145	GLU	2.1
1	Q	62	ARG	2.1
1	C	80	ILE	2.1
2	L	137	LYS	2.1
1	E	160	MET	2.1
2	T	10	MET	2.1
1	E	35	TRP	2.1
2	T	98	HIS	2.0
2	L	34	THR	2.0
1	P	203	GLY	2.0
1	C	141	VAL	2.0
2	V	11	ILE	2.0
1	E	142	LEU	2.0
1	C	144	VAL	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
4	MAN	a	5	11/12	0.49	0.84	240,308,366,376	0
4	MAN	j	6	11/12	0.54	0.34	248,304,355,371	0
4	MAN	a	4	11/12	0.64	0.45	292,310,342,361	0
5	MAN	b	5	11/12	0.65	0.35	186,281,322,333	0
5	MAN	d	4	11/12	0.65	0.34	223,300,324,344	0
3	MAN	e	5	11/12	0.66	0.27	229,267,300,324	0
4	MAN	a	6	11/12	0.69	0.44	217,289,309,314	0
3	MAN	e	4	11/12	0.71	0.22	242,274,322,327	0
5	MAN	c	5	11/12	0.73	0.24	184,249,291,304	0
4	MAN	i	7	11/12	0.73	0.32	200,242,264,268	0
4	MAN	Z	6	11/12	0.75	0.25	227,270,316,333	0
4	MAN	Z	5	11/12	0.77	0.29	219,268,297,306	0
4	MAN	i	4	11/12	0.77	0.17	268,299,347,351	0
3	MAN	h	6	11/12	0.77	0.28	214,290,327,327	0
5	MAN	c	4	11/12	0.77	0.26	222,282,306,313	0
3	MAN	f	5	11/12	0.77	0.30	165,285,305,311	0
3	MAN	h	5	11/12	0.77	0.34	294,320,348,349	0
5	BMA	c	3	11/12	0.79	0.12	239,257,278,284	0
3	MAN	Y	5	11/12	0.79	0.32	172,278,292,311	0
4	BMA	a	3	11/12	0.80	0.28	208,249,289,300	0
3	MAN	f	6	11/12	0.81	0.24	183,247,291,293	0
4	MAN	a	7	11/12	0.81	0.25	178,249,271,281	0
5	BMA	d	3	11/12	0.81	0.19	197,221,242,300	0
4	MAN	i	5	11/12	0.81	0.19	189,286,305,313	0
4	MAN	j	7	11/12	0.82	0.22	216,284,323,332	0
4	NAG	j	1	14/15	0.83	0.26	154,190,260,269	0
4	MAN	j	4	11/12	0.83	0.14	256,287,316,320	0
5	MAN	g	4	11/12	0.83	0.26	213,249,288,290	0
3	MAN	f	4	11/12	0.84	0.20	222,259,293,368	0
3	MAN	Y	6	11/12	0.84	0.23	179,283,319,340	0
4	NAG	a	2	14/15	0.85	0.30	182,258,282,287	0
3	BMA	h	3	11/12	0.85	0.17	189,230,277,279	0
5	NAG	c	1	14/15	0.85	0.22	185,254,298,308	0
4	NAG	a	1	14/15	0.85	0.19	223,276,318,345	0
4	MAN	j	5	11/12	0.85	0.25	233,279,298,326	0
5	MAN	b	4	11/12	0.85	0.30	204,256,281,283	0
4	MAN	i	6	11/12	0.86	0.29	254,324,359,371	0
4	NAG	j	2	14/15	0.86	0.29	171,184,232,241	0
5	NAG	b	2	14/15	0.87	0.24	152,204,221,276	0
5	MAN	d	5	11/12	0.87	0.27	229,290,322,341	0
3	BMA	Y	3	11/12	0.87	0.14	196,227,268,279	0
3	MAN	Y	4	11/12	0.87	0.25	215,291,309,312	0
4	MAN	Z	4	11/12	0.87	0.23	270,298,320,337	0

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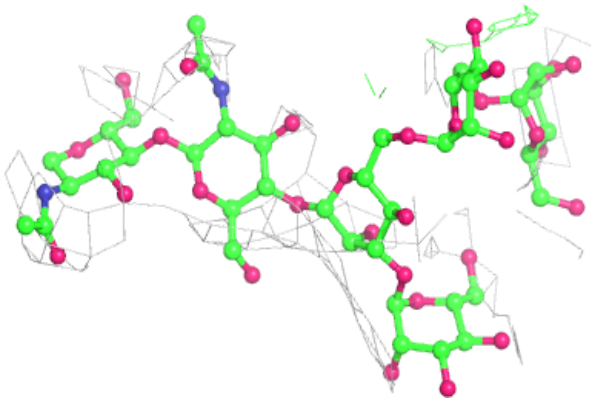
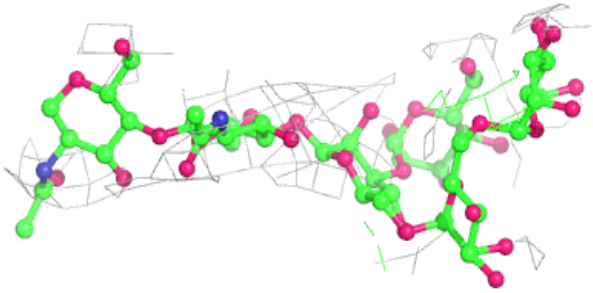
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	e	3	11/12	0.87	0.15	199,229,289,318	0
4	MAN	Z	7	11/12	0.88	0.24	186,234,277,304	0
3	MAN	e	6	11/12	0.88	0.23	159,266,328,347	0
4	BMA	i	3	11/12	0.89	0.16	175,205,224,271	0
5	BMA	b	3	11/12	0.89	0.21	191,228,274,332	0
5	NAG	c	2	14/15	0.90	0.26	206,257,279,286	0
3	NAG	h	1	14/15	0.90	0.27	129,218,239,239	0
3	MAN	h	4	11/12	0.91	0.27	235,283,301,320	0
4	NAG	i	1	14/15	0.91	0.22	172,210,247,251	0
5	MAN	g	5	11/12	0.91	0.29	172,240,270,283	0
3	NAG	f	2	14/15	0.92	0.30	113,159,214,279	0
5	NAG	d	2	14/15	0.92	0.20	154,216,246,271	0
5	NAG	b	1	14/15	0.92	0.20	202,246,270,275	0
5	NAG	d	1	14/15	0.92	0.27	194,268,287,303	0
3	NAG	e	2	14/15	0.93	0.26	157,188,237,248	0
4	NAG	i	2	14/15	0.93	0.29	148,181,242,292	0
3	NAG	f	1	14/15	0.93	0.31	101,187,221,223	0
3	BMA	f	3	11/12	0.94	0.13	122,186,227,233	0
5	BMA	g	3	11/12	0.94	0.18	202,211,256,269	0
5	NAG	g	2	14/15	0.94	0.27	147,178,203,238	0
5	NAG	g	1	14/15	0.94	0.35	164,202,282,318	0
3	NAG	h	2	14/15	0.94	0.25	109,185,229,268	0
3	NAG	Y	2	14/15	0.95	0.28	111,181,227,233	0
4	NAG	Z	1	14/15	0.95	0.24	158,192,224,246	0
4	NAG	Z	2	14/15	0.95	0.30	145,197,251,263	0
4	BMA	Z	3	11/12	0.95	0.12	176,222,235,279	0
3	NAG	Y	1	14/15	0.95	0.28	158,184,245,246	0
3	NAG	e	1	14/15	0.96	0.30	142,190,244,278	0
4	BMA	j	3	11/12	0.96	0.13	155,209,248,250	0

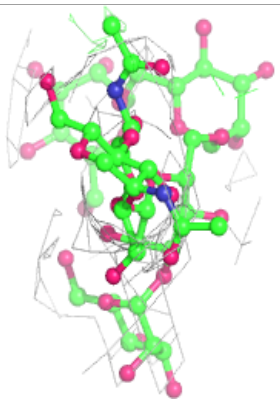
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain Y:

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

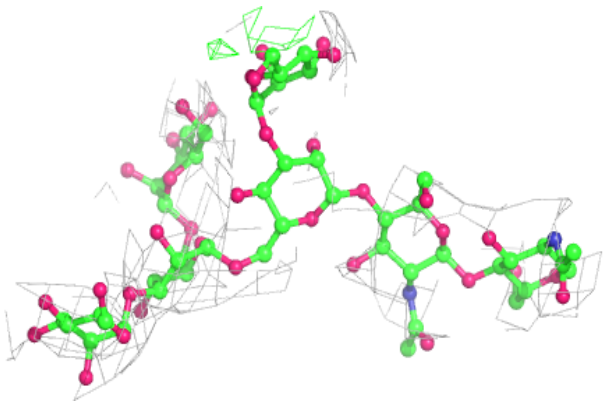


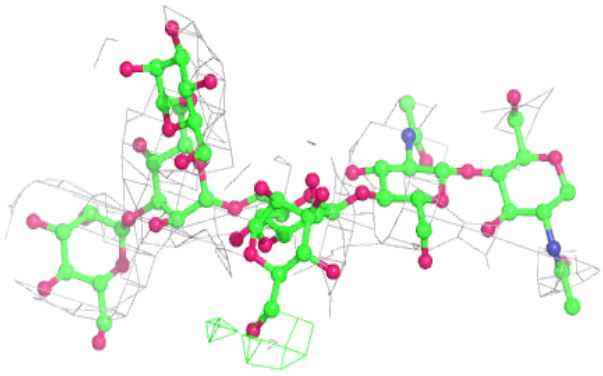


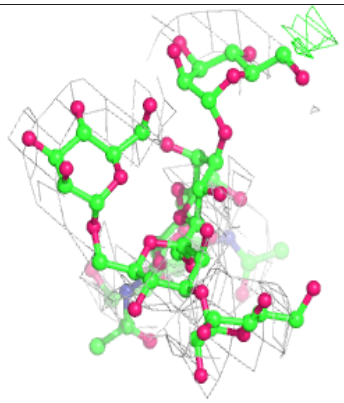


Electron density around Chain Z:

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







6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.