wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2020 – 09:01 PM BST

PDB ID	:	4R2G
Title	:	Crystal Structure of PGT124 Fab bound to HIV-1 JRCSF gp120 core and to CD4
Authors	:	Garces, F.; Wilson, I.A.
Deposited on	:	2014-08-11
Resolution	:	3.28 Å(reported)

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

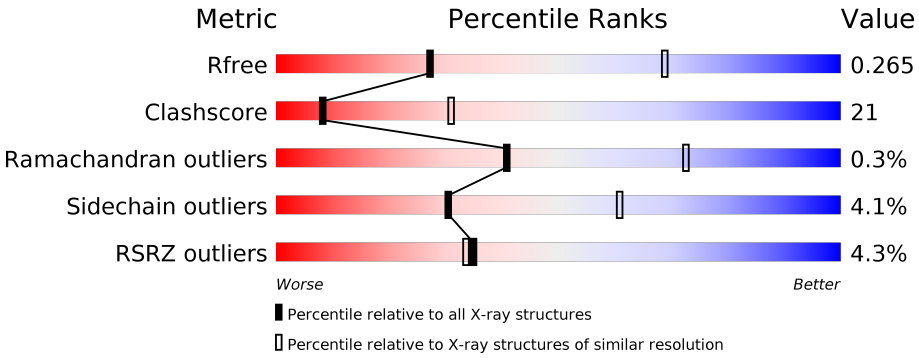
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.28 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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	309	4% 60% 34%
1	E	309	6% 65% 32%
1	K	309	6% 58% 39%
1	O	309	3% 62% 33%
2	B	184	5% 68% 26% 5%
2	F	184	12% 71% 23% 5%

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Mol	Chain	Length	Quality of chain
2	H	184	12% 66% 27%
2	L	184	10% 60% 33% 6%
3	C	214	4% 68% 27%
3	I	214	74% 24%
3	M	214	74% 21%
3	P	214	68% 26%
4	D	236	4% 53% 39% 5%
4	J	236	69% 24%
4	N	236	2% 59% 34%
4	Q	236	% 59% 34%
5	G	10	30% 60% 10%
5	R	10	20% 70% 10%
5	S	10	50% 40% 10%
5	V	10	30% 50% 20%
6	T	2	50% 50%
6	U	2	100%

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
5	MAN	S	10	-	-	X	-
5	NAG	V	1	-	-	X	-
5	MAN	V	10	-	-	X	-
5	MAN	V	7	-	-	X	-
9	GOL	D	301	-	-	X	-
9	GOL	J	301	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 29158 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 Surface protein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	303	Total	C	N	O	S	0	0	0
			2383	1491	422	451	19			
1	O	303	Total	C	N	O	S	0	0	0
			2383	1491	422	451	19			
1	A	302	Total	C	N	O	S	0	0	0
			2375	1485	421	450	19			
1	K	303	Total	C	N	O	S	0	0	0
			2383	1491	422	451	19			

There are 148 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	92	ASP	-	expression tag	UNP P20871
E	93	PHE	-	expression tag	UNP P20871
E	94	ASN	-	expression tag	UNP P20871
E	95	MET	-	expression tag	UNP P20871
E	96	TRP	-	expression tag	UNP P20871
E	97	LYS	-	expression tag	UNP P20871
E	98	ASN	-	expression tag	UNP P20871
E	99	ASN	-	expression tag	UNP P20871
E	100	MET	-	expression tag	UNP P20871
E	101	VAL	-	expression tag	UNP P20871
E	102	GLU	-	expression tag	UNP P20871
E	103	GLN	-	expression tag	UNP P20871
E	104	MET	-	expression tag	UNP P20871
E	105	GLN	-	expression tag	UNP P20871
E	106	GLU	-	expression tag	UNP P20871
E	107	ASP	-	expression tag	UNP P20871
E	108	VAL	-	expression tag	UNP P20871
E	109	ILE	-	expression tag	UNP P20871
E	110	ASN	-	expression tag	UNP P20871
E	111	LEU	-	expression tag	UNP P20871
E	112	TRP	-	expression tag	UNP P20871

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Chain	Residue	Modelled	Actual	Comment	Reference
E	113	ASP	-	expression tag	UNP P20871
E	114	GLN	-	expression tag	UNP P20871
E	115	SER	-	expression tag	UNP P20871
E	116	LEU	-	expression tag	UNP P20871
E	117	LYS	-	expression tag	UNP P20871
E	118	PRO	-	expression tag	UNP P20871
E	119	CYS	-	expression tag	UNP P20871
E	120	VAL	-	expression tag	UNP P20871
E	121	LYS	-	expression tag	UNP P20871
E	122	LEU	-	expression tag	UNP P20871
E	123	THR	-	expression tag	UNP P20871
E	197	GLY	-	expression tag	UNP P20871
E	198	GLY	-	expression tag	UNP P20871
E	317	THR	-	linker	UNP P20871
E	318	ARG	-	linker	UNP P20871
E	319	PRO	-	linker	UNP P20871
O	92	ASP	-	expression tag	UNP P20871
O	93	PHE	-	expression tag	UNP P20871
O	94	ASN	-	expression tag	UNP P20871
O	95	MET	-	expression tag	UNP P20871
O	96	TRP	-	expression tag	UNP P20871
O	97	LYS	-	expression tag	UNP P20871
O	98	ASN	-	expression tag	UNP P20871
O	99	ASN	-	expression tag	UNP P20871
O	100	MET	-	expression tag	UNP P20871
O	101	VAL	-	expression tag	UNP P20871
O	102	GLU	-	expression tag	UNP P20871
O	103	GLN	-	expression tag	UNP P20871
O	104	MET	-	expression tag	UNP P20871
O	105	GLN	-	expression tag	UNP P20871
O	106	GLU	-	expression tag	UNP P20871
O	107	ASP	-	expression tag	UNP P20871
O	108	VAL	-	expression tag	UNP P20871
O	109	ILE	-	expression tag	UNP P20871
O	110	ASN	-	expression tag	UNP P20871
O	111	LEU	-	expression tag	UNP P20871
O	112	TRP	-	expression tag	UNP P20871
O	113	ASP	-	expression tag	UNP P20871
O	114	GLN	-	expression tag	UNP P20871
O	115	SER	-	expression tag	UNP P20871
O	116	LEU	-	expression tag	UNP P20871
O	117	LYS	-	expression tag	UNP P20871

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Chain	Residue	Modelled	Actual	Comment	Reference
O	118	PRO	-	expression tag	UNP P20871
O	119	CYS	-	expression tag	UNP P20871
O	120	VAL	-	expression tag	UNP P20871
O	121	LYS	-	expression tag	UNP P20871
O	122	LEU	-	expression tag	UNP P20871
O	123	THR	-	expression tag	UNP P20871
O	197	GLY	-	expression tag	UNP P20871
O	198	GLY	-	expression tag	UNP P20871
O	317	THR	-	linker	UNP P20871
O	318	ARG	-	linker	UNP P20871
O	319	PRO	-	linker	UNP P20871
A	92	ASP	-	expression tag	UNP P20871
A	93	PHE	-	expression tag	UNP P20871
A	94	ASN	-	expression tag	UNP P20871
A	95	MET	-	expression tag	UNP P20871
A	96	TRP	-	expression tag	UNP P20871
A	97	LYS	-	expression tag	UNP P20871
A	98	ASN	-	expression tag	UNP P20871
A	99	ASN	-	expression tag	UNP P20871
A	100	MET	-	expression tag	UNP P20871
A	101	VAL	-	expression tag	UNP P20871
A	102	GLU	-	expression tag	UNP P20871
A	103	GLN	-	expression tag	UNP P20871
A	104	MET	-	expression tag	UNP P20871
A	105	GLN	-	expression tag	UNP P20871
A	106	GLU	-	expression tag	UNP P20871
A	107	ASP	-	expression tag	UNP P20871
A	108	VAL	-	expression tag	UNP P20871
A	109	ILE	-	expression tag	UNP P20871
A	110	ASN	-	expression tag	UNP P20871
A	111	LEU	-	expression tag	UNP P20871
A	112	TRP	-	expression tag	UNP P20871
A	113	ASP	-	expression tag	UNP P20871
A	114	GLN	-	expression tag	UNP P20871
A	115	SER	-	expression tag	UNP P20871
A	116	LEU	-	expression tag	UNP P20871
A	117	LYS	-	expression tag	UNP P20871
A	118	PRO	-	expression tag	UNP P20871
A	119	CYS	-	expression tag	UNP P20871
A	120	VAL	-	expression tag	UNP P20871
A	121	LYS	-	expression tag	UNP P20871
A	122	LEU	-	expression tag	UNP P20871

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Chain	Residue	Modelled	Actual	Comment	Reference
A	123	THR	-	expression tag	UNP P20871
A	197	GLY	-	expression tag	UNP P20871
A	198	GLY	-	expression tag	UNP P20871
A	317	THR	-	linker	UNP P20871
A	318	ARG	-	linker	UNP P20871
A	319	PRO	-	linker	UNP P20871
K	92	ASP	-	expression tag	UNP P20871
K	93	PHE	-	expression tag	UNP P20871
K	94	ASN	-	expression tag	UNP P20871
K	95	MET	-	expression tag	UNP P20871
K	96	TRP	-	expression tag	UNP P20871
K	97	LYS	-	expression tag	UNP P20871
K	98	ASN	-	expression tag	UNP P20871
K	99	ASN	-	expression tag	UNP P20871
K	100	MET	-	expression tag	UNP P20871
K	101	VAL	-	expression tag	UNP P20871
K	102	GLU	-	expression tag	UNP P20871
K	103	GLN	-	expression tag	UNP P20871
K	104	MET	-	expression tag	UNP P20871
K	105	GLN	-	expression tag	UNP P20871
K	106	GLU	-	expression tag	UNP P20871
K	107	ASP	-	expression tag	UNP P20871
K	108	VAL	-	expression tag	UNP P20871
K	109	ILE	-	expression tag	UNP P20871
K	110	ASN	-	expression tag	UNP P20871
K	111	LEU	-	expression tag	UNP P20871
K	112	TRP	-	expression tag	UNP P20871
K	113	ASP	-	expression tag	UNP P20871
K	114	GLN	-	expression tag	UNP P20871
K	115	SER	-	expression tag	UNP P20871
K	116	LEU	-	expression tag	UNP P20871
K	117	LYS	-	expression tag	UNP P20871
K	118	PRO	-	expression tag	UNP P20871
K	119	CYS	-	expression tag	UNP P20871
K	120	VAL	-	expression tag	UNP P20871
K	121	LYS	-	expression tag	UNP P20871
K	122	LEU	-	expression tag	UNP P20871
K	123	THR	-	expression tag	UNP P20871
K	197	GLY	-	expression tag	UNP P20871
K	198	GLY	-	expression tag	UNP P20871
K	317	THR	-	linker	UNP P20871
K	318	ARG	-	linker	UNP P20871

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Chain	Residue	Modelled	Actual	Comment	Reference
K	319	PRO	-	linker	UNP P20871

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	175	Total	C	N	O	S	0	0	0
			1363	851	239	269	4			
2	B	175	Total	C	N	O	S	0	0	0
			1363	851	239	269	4			
2	H	176	Total	C	N	O	S	0	0	0
			1368	854	240	270	4			
2	L	173	Total	C	N	O	S	0	0	0
			1345	839	235	267	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	MET	-	initiating methionine	UNP P01730
B	0	MET	-	initiating methionine	UNP P01730
H	0	MET	-	initiating methionine	UNP P01730
L	0	MET	-	initiating methionine	UNP P01730

- Molecule 3 is a protein called PGT124 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	210	Total	C	N	O	S	0	0	0
			1595	1005	270	315	5			
3	C	210	Total	C	N	O	S	0	0	0
			1595	1005	270	315	5			
3	I	210	Total	C	N	O	S	0	0	0
			1595	1005	270	315	5			
3	M	210	Total	C	N	O	S	0	0	0
			1595	1005	270	315	5			

- Molecule 4 is a protein called PGT124 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Q	228	Total	C	N	O	S	0	0	0
			1732	1099	289	339	5			
4	D	225	Total	C	N	O	S	0	0	0
			1716	1091	286	334	5			

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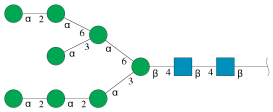
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	226	Total	C	N	O	S	0	0	0
			1720	1093	287	335	5			
4	N	228	Total	C	N	O	S	0	0	0
			1735	1101	290	339	5			

- Molecule 5 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.

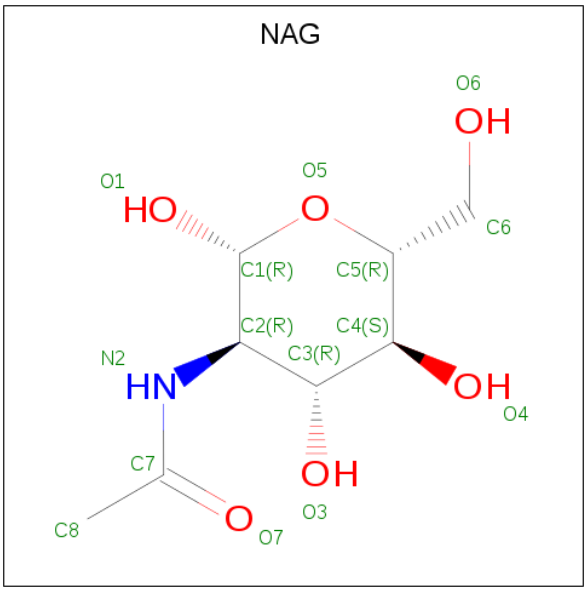


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	10	Total	C	N	O	0	0	0
			116	64	2	50			
5	R	10	Total	C	N	O	0	0	0
			116	64	2	50			
5	S	10	Total	C	N	O	0	0	0
			116	64	2	50			
5	V	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 6 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
6	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	U	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total C N O 14 8 1 5	0	0
7	E	1	Total C N O 14 8 1 5	0	0
7	E	1	Total C N O 14 8 1 5	0	0
7	E	1	Total C N O 14 8 1 5	0	0
7	E	1	Total C N O 14 8 1 5	0	0
7	E	1	Total C N O 14 8 1 5	0	0
7	E	1	Total C N O 14 8 1 5	0	0
7	E	1	Total C N O 14 8 1 5	0	0
7	O	1	Total C N O 14 8 1 5	0	0
7	O	1	Total C N O 14 8 1 5	0	0
7	O	1	Total C N O 14 8 1 5	0	0
7	O	1	Total C N O 14 8 1 5	0	0
7	O	1	Total C N O 14 8 1 5	0	0
7	O	1	Total C N O 14 8 1 5	0	0

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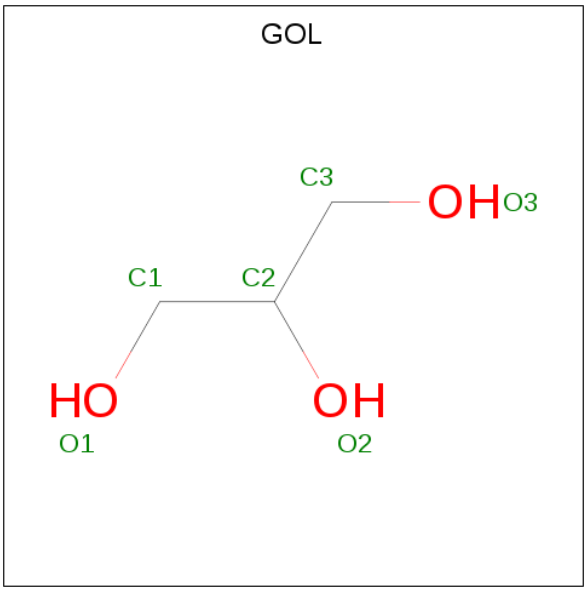
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	O	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	K	1	Total C N O 14 8 1 5	0	0
7	K	1	Total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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	O	1	Total Cl 1 1	0	0
8	A	1	Total Cl 1 1	0	0
8	K	1	Total Cl 1 1	0	0
8	E	1	Total Cl 1 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



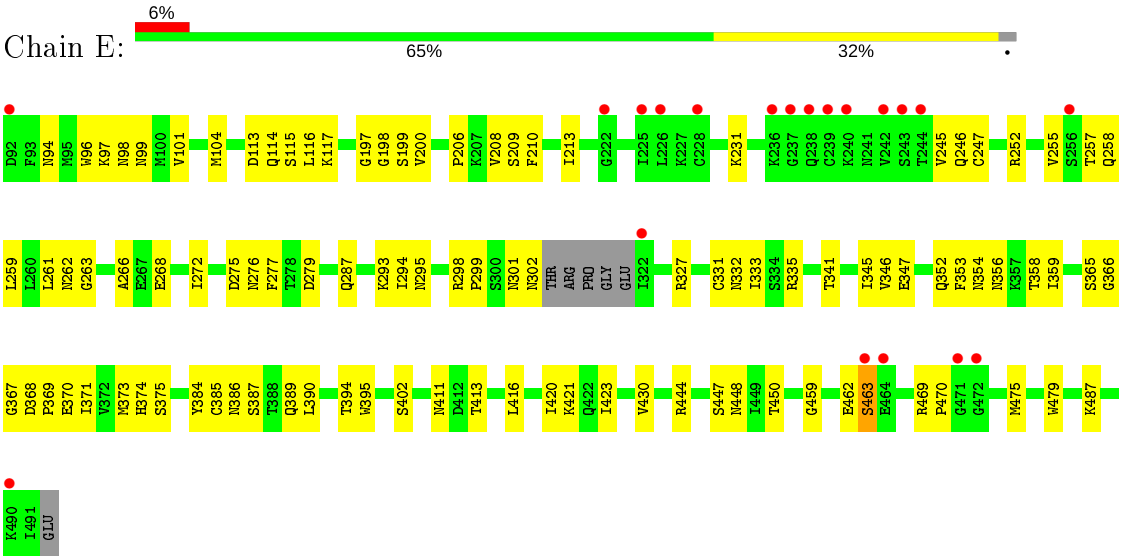
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	Q	1	Total	C	O	0	0
			6	3	3		
9	D	1	Total	C	O	0	0
			6	3	3		
9	J	1	Total	C	O	0	0
			6	3	3		
9	N	1	Total	C	O	0	0
			6	3	3		

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.

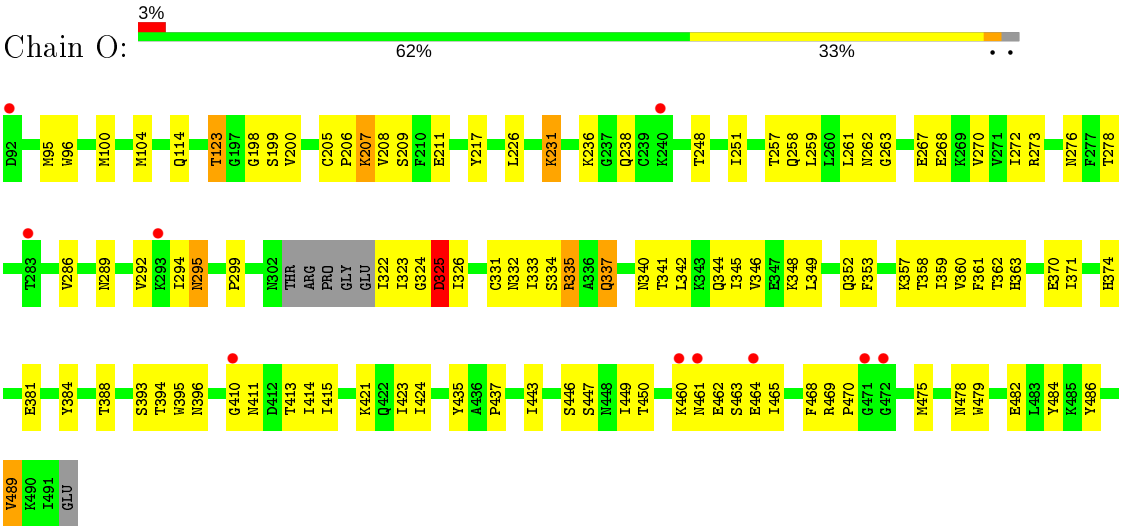
- Molecule 1: Surface protein gp160

Chain E:



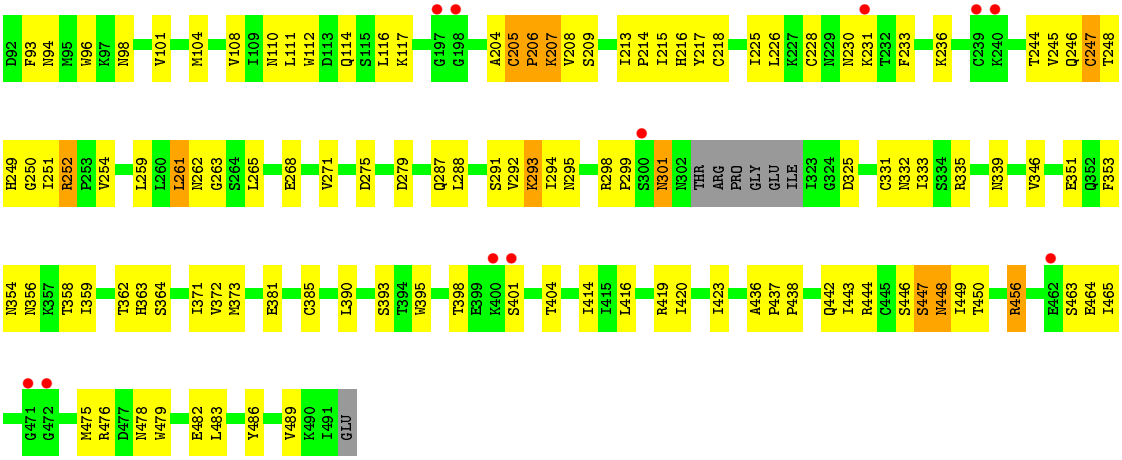
- Molecule 1: Surface protein gp160

Chain O:



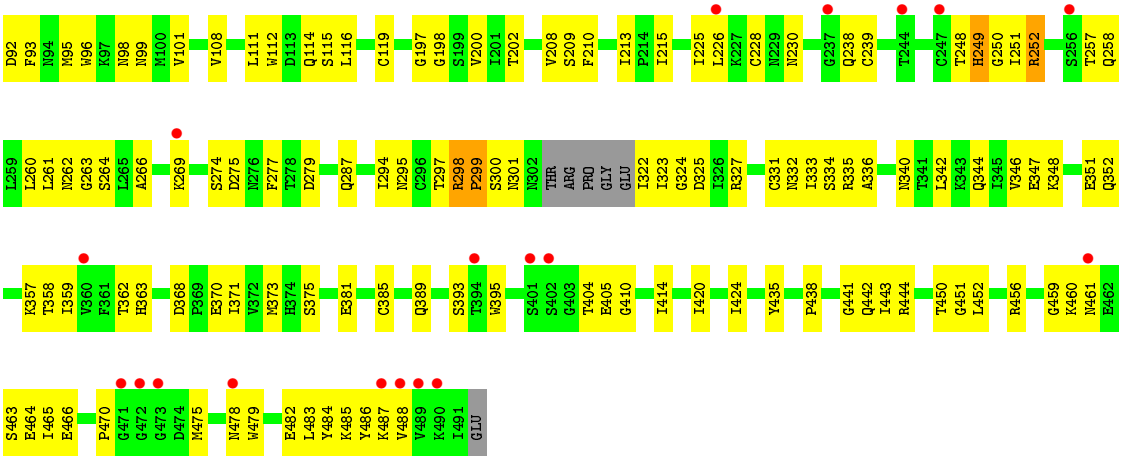
- Molecule 1: Surface protein gp160

Chain A:



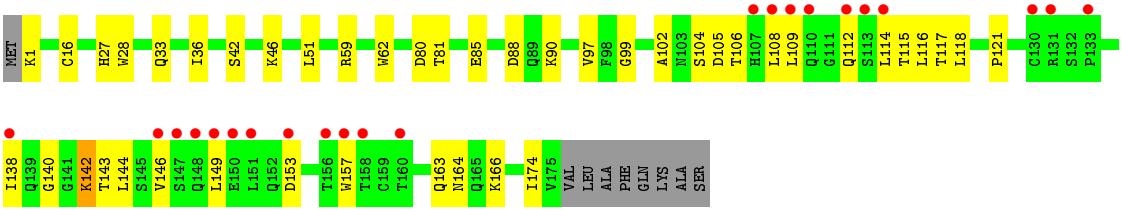
• Molecule 1: Surface protein gp160

Chain K:



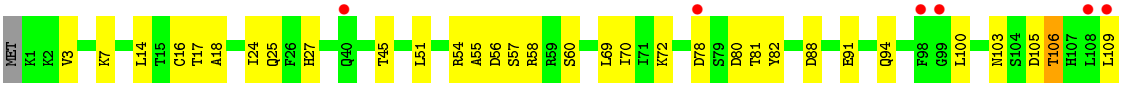
• Molecule 2: T-cell surface glycoprotein CD4

Chain F:



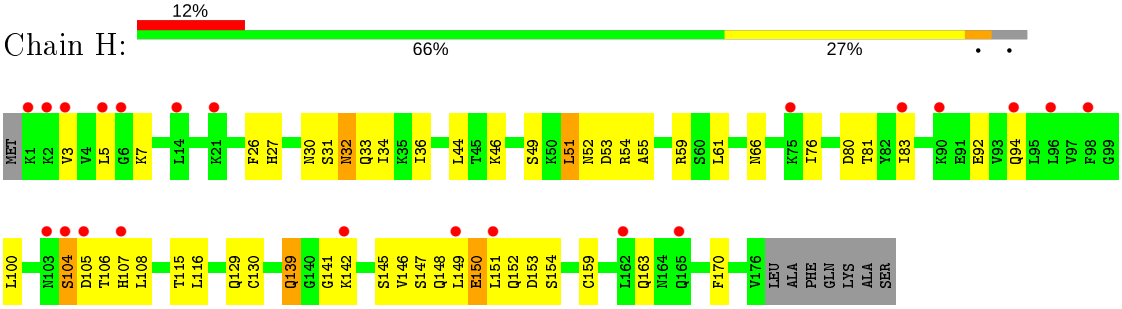
• Molecule 2: T-cell surface glycoprotein CD4

Chain B:



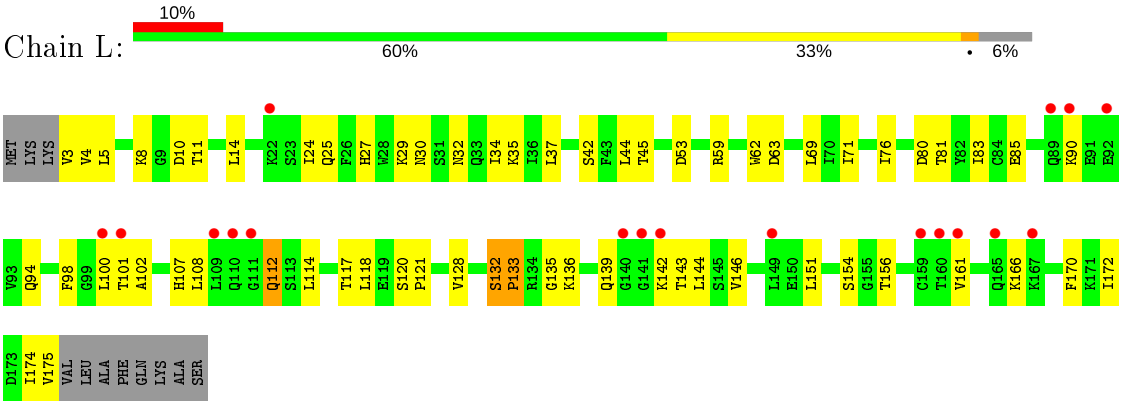
- Molecule 2: T-cell surface glycoprotein CD4

Chain H:



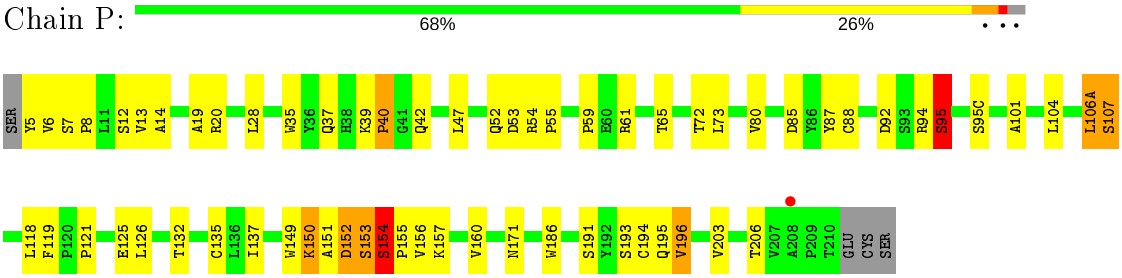
- Molecule 2: T-cell surface glycoprotein CD4

Chain L:



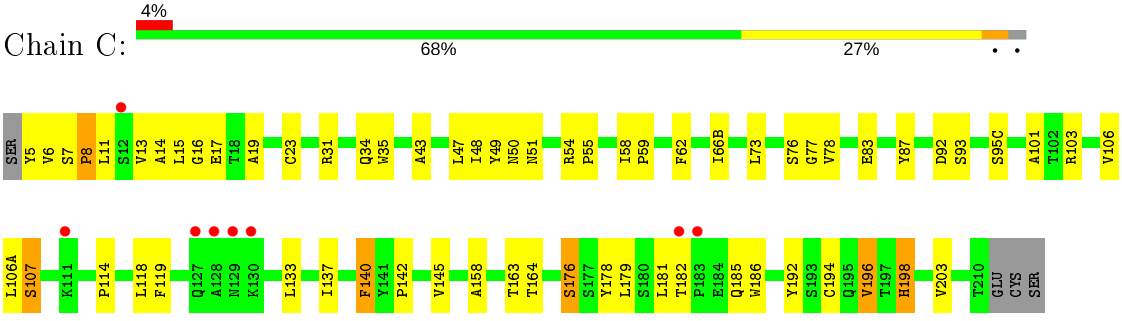
- Molecule 3: PGT124 Light Chain

Chain P:



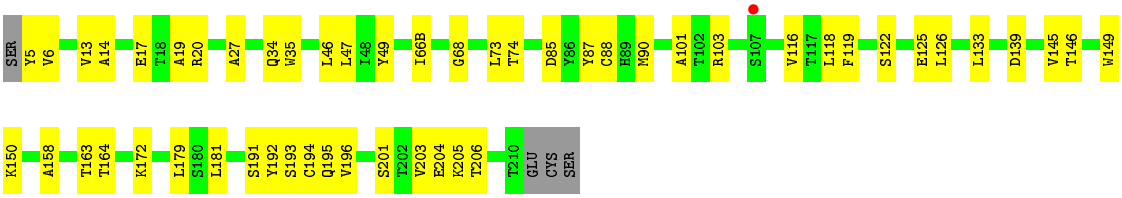
- Molecule 3: PGT124 Light Chain

Chain C:



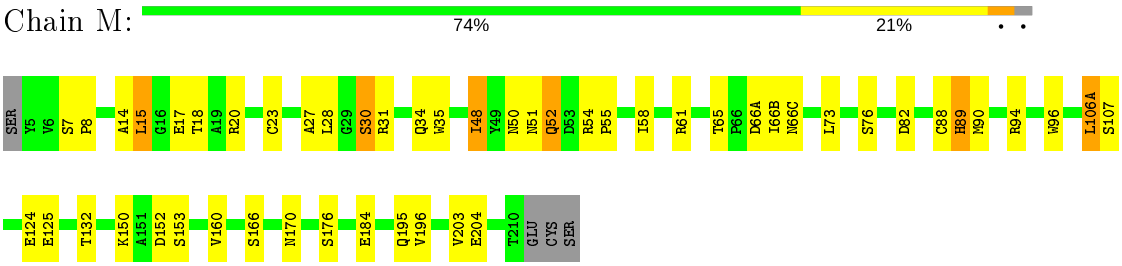
• Molecule 3: PGT124 Light Chain

Chain I:



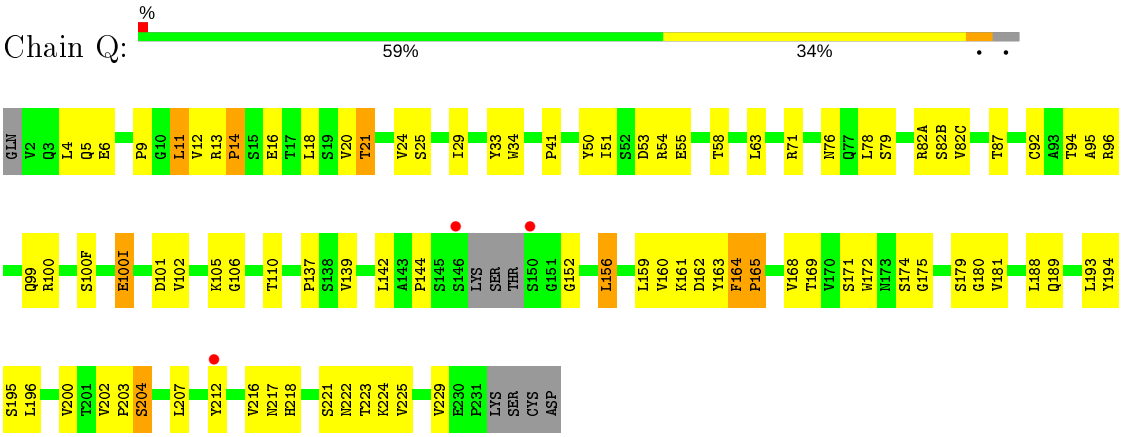
• Molecule 3: PGT124 Light Chain

Chain M:



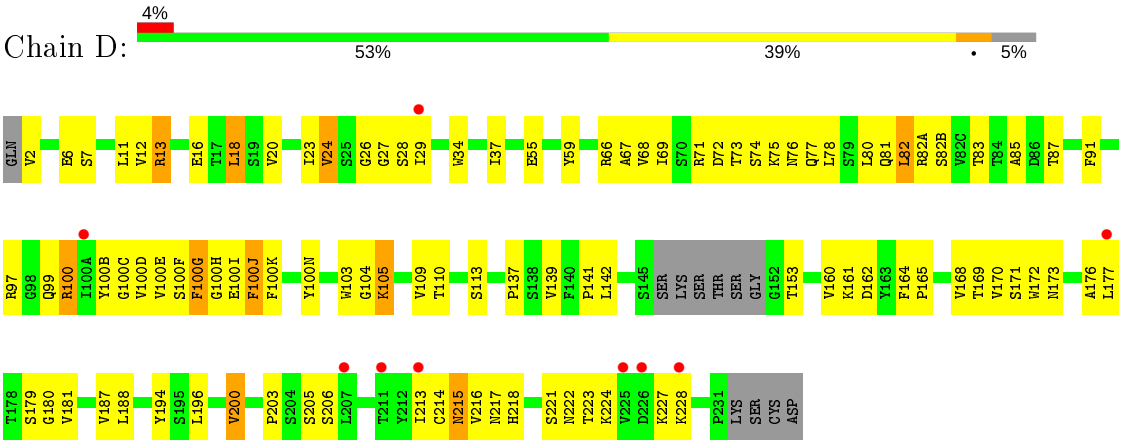
• Molecule 4: PGT124 Heavy Chain

Chain Q:



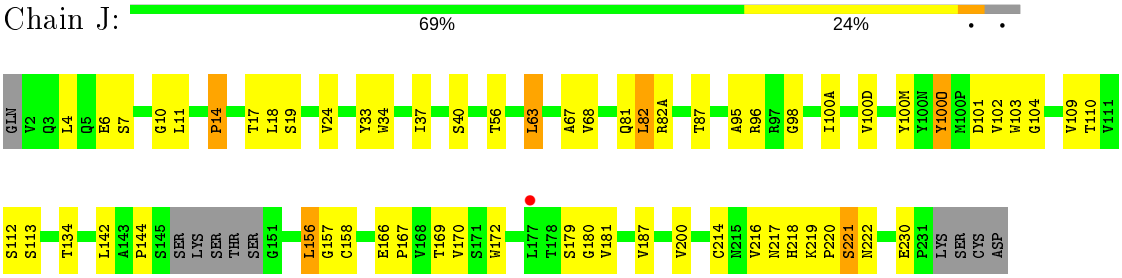
• Molecule 4: PGT124 Heavy Chain

Chain D:



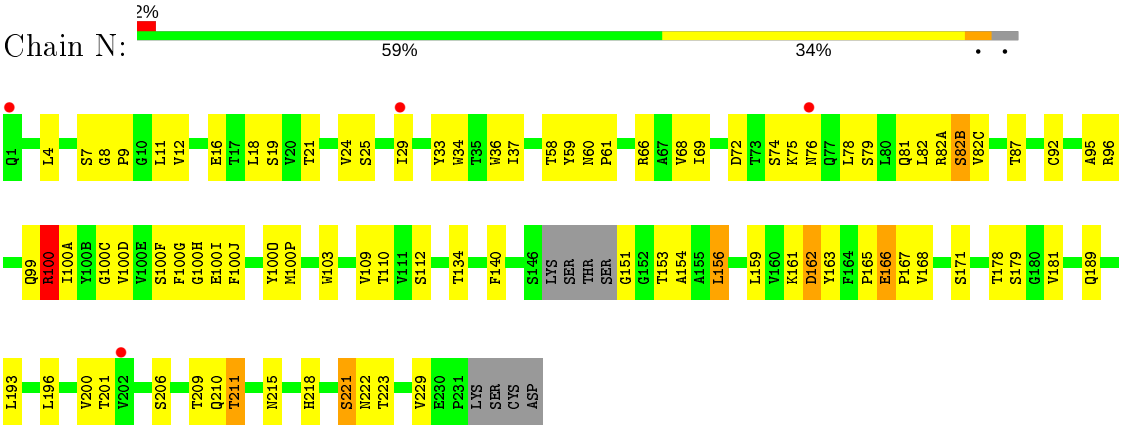
• Molecule 4: PGT124 Heavy Chain

Chain J:



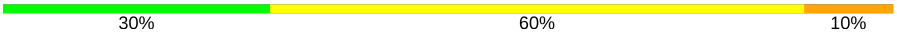
• Molecule 4: PGT124 Heavy Chain

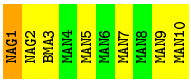
Chain N:



• Molecule 5: 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

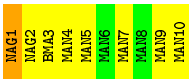
Chain G:





• Molecule 5: 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 R:



• Molecule 5: 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 S:

• Molecule 5: 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

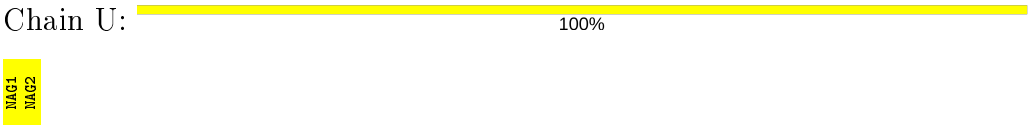
Chain V:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	164.41Å 165.44Å 229.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.65 – 3.28 39.65 – 3.28	Depositor EDS
% Data completeness (in resolution range)	98.4 (39.65-3.28) 98.5 (39.65-3.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.207 , 0.263 0.210 , 0.265	Depositor DCC
R_{free} test set	4722 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	94.1	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	29158	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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: GOL, CL, 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	0.38	1/2419 (0.0%)	0.60	2/3268 (0.1%)
1	E	0.40	1/2427 (0.0%)	0.61	1/3279 (0.0%)
1	K	0.35	1/2427 (0.0%)	0.60	2/3279 (0.1%)
1	O	0.36	0/2427	0.56	0/3279
2	B	0.32	0/1382	0.54	0/1863
2	F	0.34	0/1382	0.59	0/1863
2	H	0.33	1/1387 (0.1%)	0.59	3/1870 (0.2%)
2	L	0.31	1/1364 (0.1%)	0.53	1/1841 (0.1%)
3	C	0.37	1/1638 (0.1%)	0.61	1/2238 (0.0%)
3	I	0.38	0/1638	0.61	0/2238
3	M	0.43	0/1638	0.67	1/2238 (0.0%)
3	P	0.53	2/1638 (0.1%)	0.71	4/2238 (0.2%)
4	D	0.39	0/1759	0.66	3/2402 (0.1%)
4	J	0.41	1/1763 (0.1%)	0.66	2/2407 (0.1%)
4	N	0.51	2/1778 (0.1%)	0.74	4/2427 (0.2%)
4	Q	0.46	1/1775 (0.1%)	0.68	2/2423 (0.1%)
All	All	0.40	12/28842 (0.0%)	0.63	26/39153 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	M	0	1
3	P	0	2
All	All	0	3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	40	PRO	N-CD	11.64	1.64	1.47
4	N	100	ARG	CA-C	-8.85	1.29	1.52
3	C	8	PRO	N-CD	-5.79	1.39	1.47
1	A	206	PRO	N-CD	5.63	1.55	1.47
1	K	299	PRO	N-CD	5.29	1.55	1.47

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Q	14	PRO	N-CA-C	8.06	133.06	112.10
3	P	107	SER	N-CA-C	-6.74	92.79	111.00
4	N	100	ARG	C-N-CA	-6.55	105.33	121.70
4	D	74	SER	N-CA-CB	6.48	120.22	110.50
3	P	40	PRO	CA-N-CD	-6.45	102.47	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	106(A)	LEU	Peptide
3	P	106(A)	LEU	Peptide
3	P	95	SER	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2375	0	2335	136	0
1	E	2383	0	2342	96	0
1	K	2383	0	2350	180	0
1	O	2383	0	2342	119	0
2	B	1363	0	1389	41	0
2	F	1363	0	1389	40	0
2	H	1368	0	1391	64	0
2	L	1345	0	1360	47	0
3	C	1595	0	1541	54	0
3	I	1595	0	1543	37	0
3	M	1595	0	1541	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	1595	0	1540	64	0
4	D	1716	0	1683	94	0
4	J	1720	0	1686	45	0
4	N	1735	0	1702	62	0
4	Q	1732	0	1696	81	0
5	G	116	0	96	11	0
5	R	116	0	96	17	0
5	S	116	0	96	13	0
5	V	116	0	96	28	0
6	T	28	0	25	1	0
6	U	28	0	25	5	0
7	A	84	0	78	7	0
7	E	112	0	104	3	0
7	K	70	0	65	4	0
7	O	98	0	91	6	0
8	A	1	0	0	0	0
8	E	1	0	0	1	0
8	K	1	0	0	1	0
8	O	1	0	0	0	0
9	D	6	0	8	5	0
9	J	6	0	8	14	0
9	N	6	0	8	3	0
9	Q	6	0	8	0	0
All	All	29158	0	28634	1214	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 21.

The worst 5 of 1214 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:332:ASN:ND2	5:V:1:NAG:H82	1.26	1.44
3:P:150:LYS:CB	3:P:193:SER:OG	1.64	1.41
7:O:515:NAG:H62	7:O:516:NAG:C8	1.51	1.38
9:J:301:GOL:H32	5:V:7:MAN:C2	1.60	1.32
1:K:335:ARG:NE	1:K:410:GLY:HA3	1.48	1.29

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	298/309 (96%)	276 (93%)	20 (7%)	2 (1%)	22	56
1	E	299/309 (97%)	272 (91%)	27 (9%)	0	100	100
1	K	299/309 (97%)	275 (92%)	23 (8%)	1 (0%)	41	72
1	O	299/309 (97%)	279 (93%)	17 (6%)	3 (1%)	15	48
2	B	173/184 (94%)	164 (95%)	8 (5%)	1 (1%)	25	58
2	F	173/184 (94%)	164 (95%)	9 (5%)	0	100	100
2	H	174/184 (95%)	157 (90%)	16 (9%)	1 (1%)	25	58
2	L	171/184 (93%)	160 (94%)	11 (6%)	0	100	100
3	C	208/214 (97%)	191 (92%)	17 (8%)	0	100	100
3	I	208/214 (97%)	186 (89%)	22 (11%)	0	100	100
3	M	208/214 (97%)	198 (95%)	10 (5%)	0	100	100
3	P	208/214 (97%)	194 (93%)	12 (6%)	2 (1%)	15	48
4	D	221/236 (94%)	197 (89%)	23 (10%)	1 (0%)	29	62
4	J	222/236 (94%)	209 (94%)	12 (5%)	1 (0%)	29	62
4	N	224/236 (95%)	206 (92%)	18 (8%)	0	100	100
4	Q	224/236 (95%)	204 (91%)	20 (9%)	0	100	100
All	All	3609/3772 (96%)	3332 (92%)	265 (7%)	12 (0%)	41	72

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	100(J)	PHE
1	A	205	CYS
1	O	231	LYS
2	B	106	THR
2	H	150	GLU

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	270/276 (98%)	260 (96%)	10 (4%)	34	62
1	E	271/276 (98%)	264 (97%)	7 (3%)	46	71
1	K	271/276 (98%)	263 (97%)	8 (3%)	41	68
1	O	271/276 (98%)	263 (97%)	8 (3%)	41	68
2	B	159/166 (96%)	157 (99%)	2 (1%)	69	82
2	F	159/166 (96%)	154 (97%)	5 (3%)	40	67
2	H	159/166 (96%)	155 (98%)	4 (2%)	47	72
2	L	157/166 (95%)	151 (96%)	6 (4%)	33	62
3	C	176/180 (98%)	169 (96%)	7 (4%)	31	61
3	I	176/180 (98%)	173 (98%)	3 (2%)	60	78
3	M	176/180 (98%)	164 (93%)	12 (7%)	16	44
3	P	176/180 (98%)	166 (94%)	10 (6%)	20	51
4	D	194/204 (95%)	180 (93%)	14 (7%)	14	41
4	J	194/204 (95%)	183 (94%)	11 (6%)	20	51
4	N	196/204 (96%)	182 (93%)	14 (7%)	14	42
4	Q	196/204 (96%)	185 (94%)	11 (6%)	21	51
All	All	3201/3304 (97%)	3069 (96%)	132 (4%)	30	61

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	147	SER
4	J	230	GLU
1	A	447	SER
3	I	181	LEU
4	J	63	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	198	HIS
4	D	76	ASN
3	M	52	GLN
2	B	33	GLN
2	B	103	ASN

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)

44 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	$\#\|Z\|>2$
5	NAG	G	1	1,5	14,14,15	0.31	0	17,19,21	0.88	1 (5%)
5	MAN	G	10	5	11,11,12	0.23	0	15,15,17	0.67	0
5	NAG	G	2	5	14,14,15	0.36	0	17,19,21	0.98	0
5	BMA	G	3	5	11,11,12	1.51	3 (27%)	15,15,17	4.28	4 (26%)
5	MAN	G	4	5	11,11,12	0.25	0	15,15,17	0.76	0
5	MAN	G	5	5	11,11,12	0.32	0	15,15,17	0.71	0
5	MAN	G	6	5	11,11,12	0.28	0	15,15,17	0.71	0
5	MAN	G	7	5	11,11,12	0.22	0	15,15,17	0.79	0
5	MAN	G	8	5	11,11,12	0.27	0	15,15,17	0.80	0
5	MAN	G	9	5	11,11,12	0.24	0	15,15,17	0.69	0
5	NAG	R	1	1,5	14,14,15	0.32	0	17,19,21	0.89	1 (5%)
5	MAN	R	10	5	11,11,12	0.24	0	15,15,17	0.66	0
5	NAG	R	2	5	14,14,15	0.37	0	17,19,21	0.97	0
5	BMA	R	3	5	11,11,12	1.51	3 (27%)	15,15,17	4.28	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	R	4	5	11,11,12	0.28	0	15,15,17	0.63	0
5	MAN	R	5	5	11,11,12	0.29	0	15,15,17	0.72	0
5	MAN	R	6	5	11,11,12	0.31	0	15,15,17	0.69	0
5	MAN	R	7	5	11,11,12	0.23	0	15,15,17	0.78	0
5	MAN	R	8	5	11,11,12	0.28	0	15,15,17	0.80	0
5	MAN	R	9	5	11,11,12	0.25	0	15,15,17	0.70	0
5	NAG	S	1	1,5	14,14,15	0.32	0	17,19,21	0.89	1 (5%)
5	MAN	S	10	5	11,11,12	0.24	0	15,15,17	0.66	0
5	NAG	S	2	5	14,14,15	0.37	0	17,19,21	0.96	0
5	BMA	S	3	5	11,11,12	1.50	3 (27%)	15,15,17	4.27	4 (26%)
5	MAN	S	4	5	11,11,12	0.24	0	15,15,17	0.75	0
5	MAN	S	5	5	11,11,12	0.28	0	15,15,17	0.73	0
5	MAN	S	6	5	11,11,12	0.31	0	15,15,17	0.69	0
5	MAN	S	7	5	11,11,12	0.23	0	15,15,17	0.78	0
5	MAN	S	8	5	11,11,12	0.28	0	15,15,17	0.80	0
5	MAN	S	9	5	11,11,12	0.24	0	15,15,17	0.70	0
6	NAG	T	1	1,6	14,14,15	0.35	0	17,19,21	0.65	0
6	NAG	T	2	6	14,14,15	0.33	0	17,19,21	0.84	1 (5%)
6	NAG	U	1	1,6	14,14,15	0.30	0	17,19,21	0.61	0
6	NAG	U	2	6	14,14,15	0.29	0	17,19,21	0.61	0
5	NAG	V	1	1,5	14,14,15	0.32	0	17,19,21	0.88	1 (5%)
5	MAN	V	10	5	11,11,12	0.22	0	15,15,17	0.66	0
5	NAG	V	2	5	14,14,15	0.36	0	17,19,21	0.97	0
5	BMA	V	3	5	11,11,12	1.51	3 (27%)	15,15,17	4.27	4 (26%)
5	MAN	V	4	5	11,11,12	0.28	0	15,15,17	0.64	0
5	MAN	V	5	5	11,11,12	0.28	0	15,15,17	0.73	0
5	MAN	V	6	5	11,11,12	0.31	0	15,15,17	0.69	0
5	MAN	V	7	5	11,11,12	0.23	0	15,15,17	0.78	0
5	MAN	V	8	5	11,11,12	0.27	0	15,15,17	0.81	0
5	MAN	V	9	5	11,11,12	0.25	0	15,15,17	0.70	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
5	NAG	G	1	1,5	-	3/6/23/26	0/1/1/1
5	MAN	G	10	5	-	0/2/19/22	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	G	4	5	-	2/2/19/22	0/1/1/1
5	MAN	G	5	5	-	2/2/19/22	0/1/1/1
5	MAN	G	6	5	-	2/2/19/22	0/1/1/1
5	MAN	G	7	5	-	0/2/19/22	0/1/1/1
5	MAN	G	8	5	-	2/2/19/22	0/1/1/1
5	MAN	G	9	5	-	2/2/19/22	0/1/1/1
5	NAG	R	1	1,5	-	3/6/23/26	0/1/1/1
5	MAN	R	10	5	-	0/2/19/22	0/1/1/1
5	NAG	R	2	5	-	1/6/23/26	0/1/1/1
5	BMA	R	3	5	-	0/2/19/22	0/1/1/1
5	MAN	R	4	5	-	0/2/19/22	0/1/1/1
5	MAN	R	5	5	-	2/2/19/22	0/1/1/1
5	MAN	R	6	5	-	2/2/19/22	0/1/1/1
5	MAN	R	7	5	-	0/2/19/22	0/1/1/1
5	MAN	R	8	5	-	2/2/19/22	0/1/1/1
5	MAN	R	9	5	-	2/2/19/22	0/1/1/1
5	NAG	S	1	1,5	-	3/6/23/26	0/1/1/1
5	MAN	S	10	5	-	0/2/19/22	0/1/1/1
5	NAG	S	2	5	-	1/6/23/26	0/1/1/1
5	BMA	S	3	5	-	0/2/19/22	0/1/1/1
5	MAN	S	4	5	-	2/2/19/22	0/1/1/1
5	MAN	S	5	5	-	2/2/19/22	0/1/1/1
5	MAN	S	6	5	-	2/2/19/22	0/1/1/1
5	MAN	S	7	5	-	0/2/19/22	0/1/1/1
5	MAN	S	8	5	-	2/2/19/22	0/1/1/1
5	MAN	S	9	5	-	2/2/19/22	0/1/1/1
6	NAG	T	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	T	2	6	-	5/6/23/26	0/1/1/1
6	NAG	U	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	U	2	6	-	3/6/23/26	0/1/1/1
5	NAG	V	1	1,5	-	3/6/23/26	0/1/1/1
5	MAN	V	10	5	-	0/2/19/22	0/1/1/1
5	NAG	V	2	5	-	1/6/23/26	0/1/1/1
5	BMA	V	3	5	-	0/2/19/22	0/1/1/1
5	MAN	V	4	5	-	0/2/19/22	0/1/1/1
5	MAN	V	5	5	-	2/2/19/22	0/1/1/1
5	MAN	V	6	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	V	7	5	-	0/2/19/22	0/1/1/1
5	MAN	V	8	5	-	2/2/19/22	0/1/1/1
5	MAN	V	9	5	-	2/2/19/22	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	3	BMA	O5-C1	2.67	1.48	1.43
5	R	3	BMA	O5-C1	2.65	1.48	1.43
5	V	3	BMA	O5-C1	2.65	1.47	1.43
5	G	3	BMA	O5-C1	2.62	1.47	1.43
5	V	3	BMA	O2-C2	-2.14	1.38	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	3	BMA	O3-C3-C2	-12.59	85.88	109.99
5	R	3	BMA	O3-C3-C2	-12.56	85.94	109.99
5	V	3	BMA	O3-C3-C2	-12.55	85.95	109.99
5	S	3	BMA	O3-C3-C2	-12.55	85.96	109.99
5	G	3	BMA	O3-C3-C4	9.50	132.32	110.35

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1	NAG	C3-C2-N2-C7
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	V	1	NAG	C3-C2-N2-C7
5	V	1	NAG	C8-C7-N2-C2

There are no ring outliers.

28 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1	NAG	4	0
5	R	5	MAN	1	0
5	V	1	NAG	8	0
5	R	2	NAG	4	0

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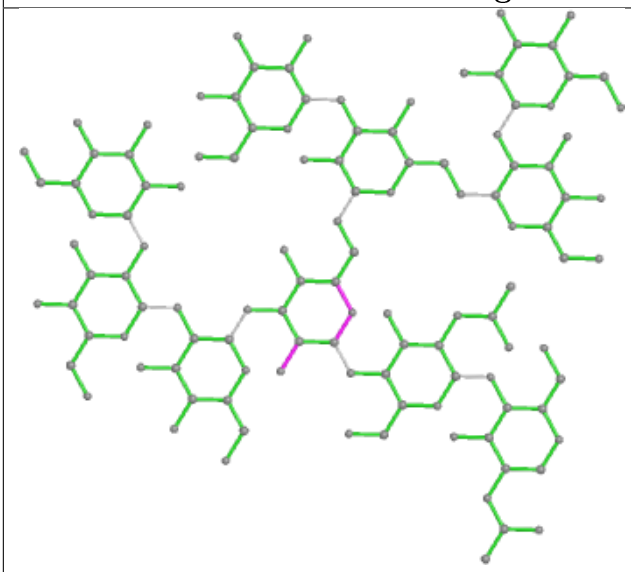
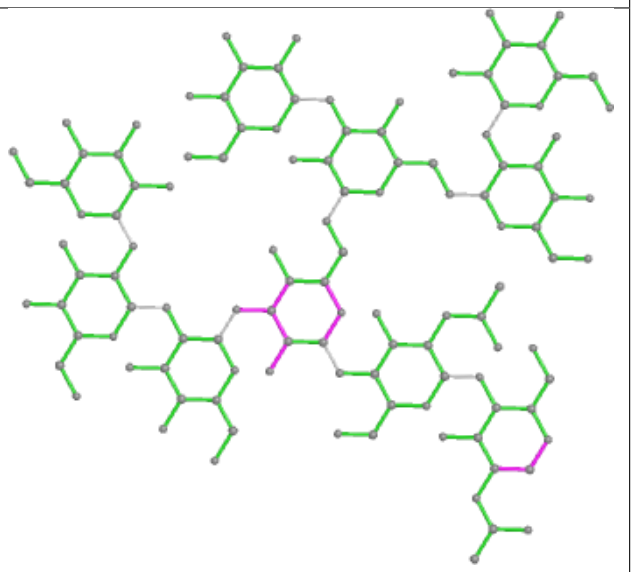
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	7	MAN	5	0
5	G	10	MAN	4	0
5	R	4	MAN	1	0
5	S	1	NAG	6	0
5	R	9	MAN	1	0
5	V	10	MAN	9	0
5	V	7	MAN	13	0
5	G	7	MAN	4	0
6	T	2	NAG	1	0
5	V	4	MAN	1	0
5	G	5	MAN	1	0
6	U	2	NAG	1	0
6	T	1	NAG	1	0
5	R	10	MAN	5	0
5	R	1	NAG	6	0
5	G	9	MAN	2	0
5	V	5	MAN	1	0
5	V	2	NAG	1	0
5	S	7	MAN	4	0
5	S	10	MAN	6	0
5	S	2	NAG	2	0
6	U	1	NAG	5	0
5	V	3	BMA	1	0
5	G	2	NAG	1	0

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

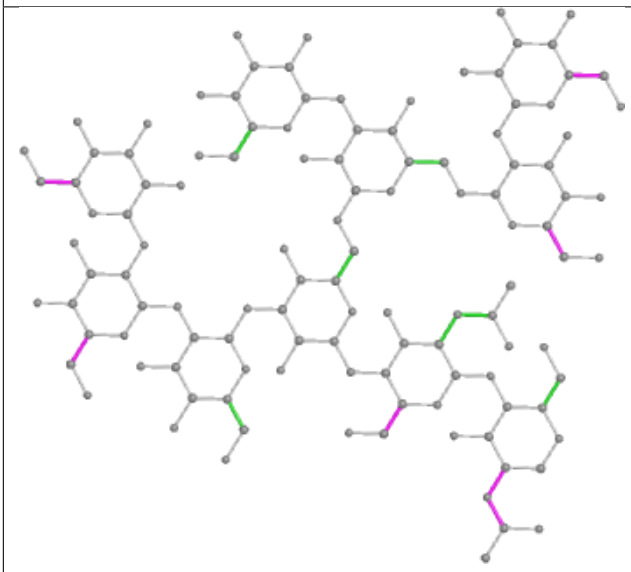
Oligosaccharide Chain R



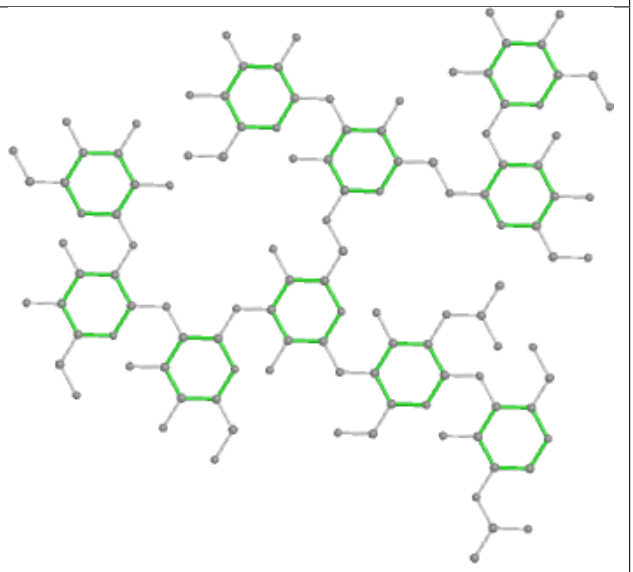
Bond lengths



Bond angles

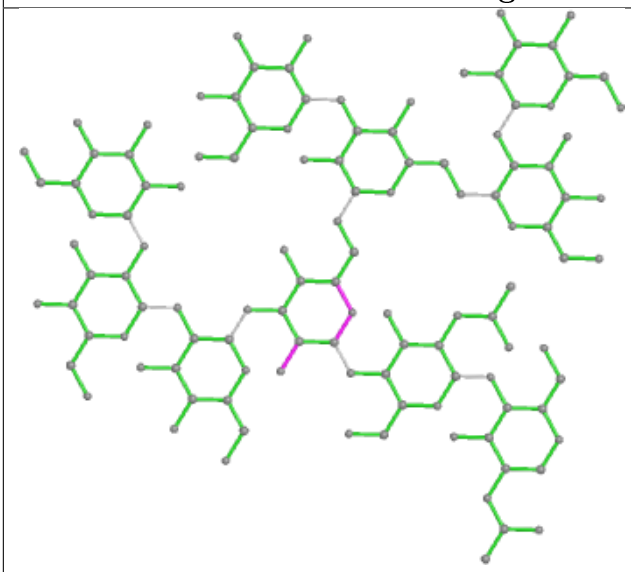


Torsions

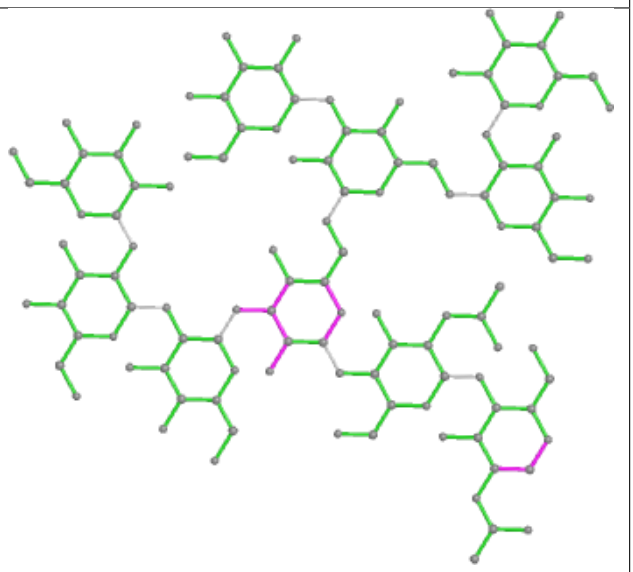


Rings

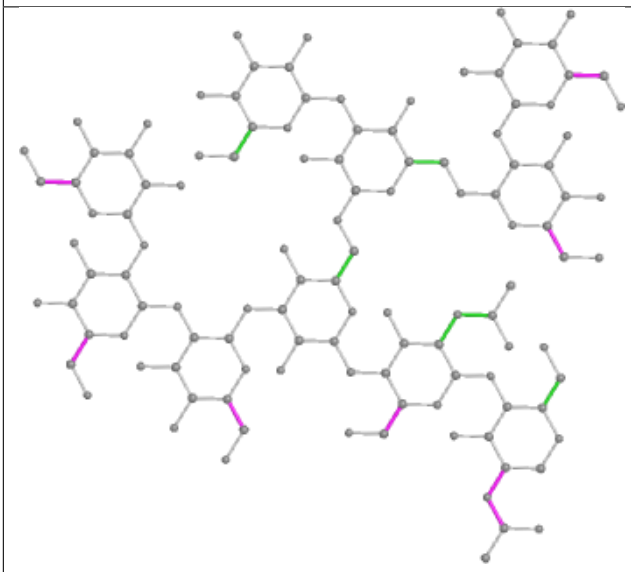
Oligosaccharide Chain S



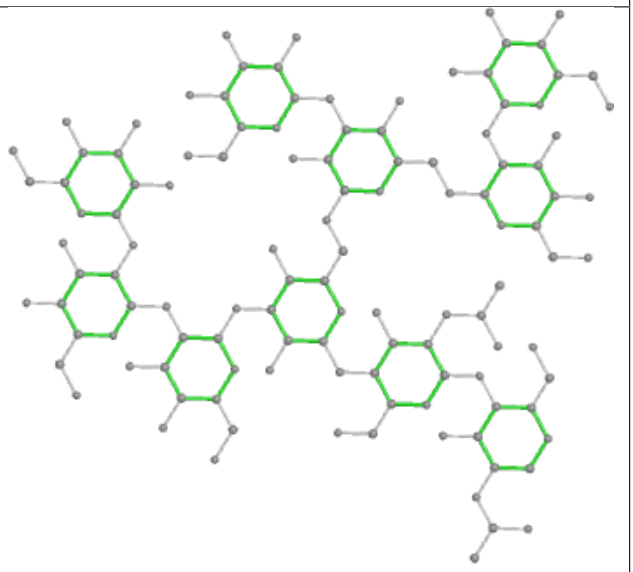
Bond lengths



Bond angles

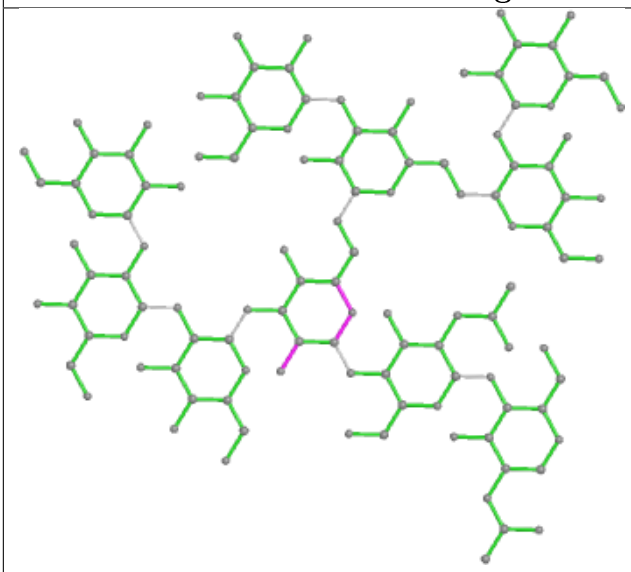


Torsions

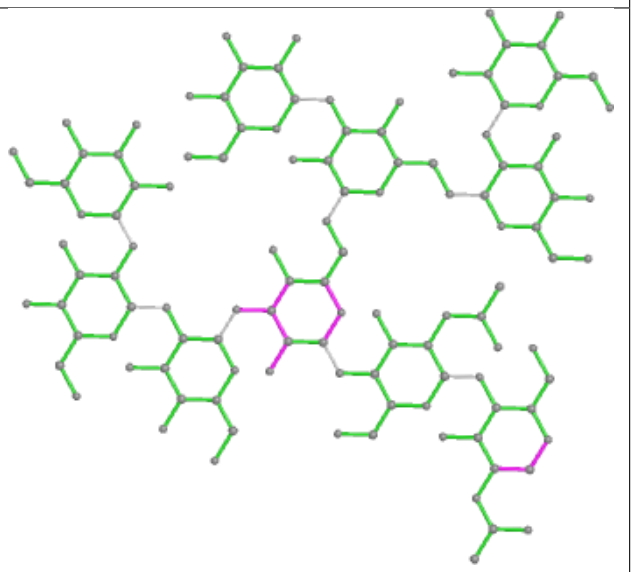


Rings

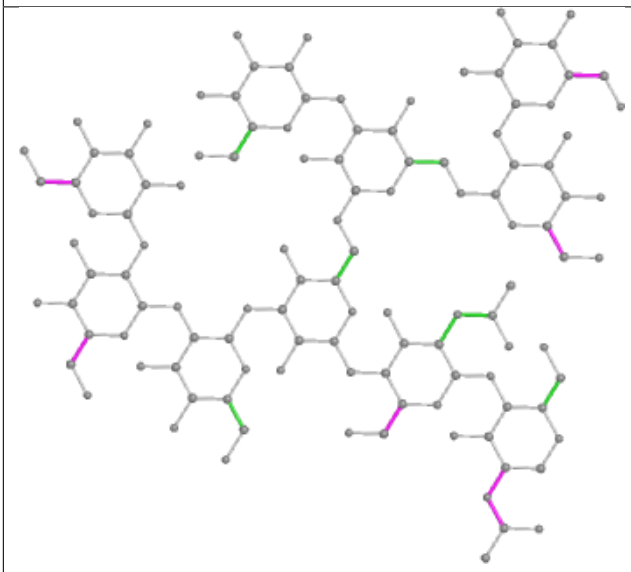
Oligosaccharide Chain V



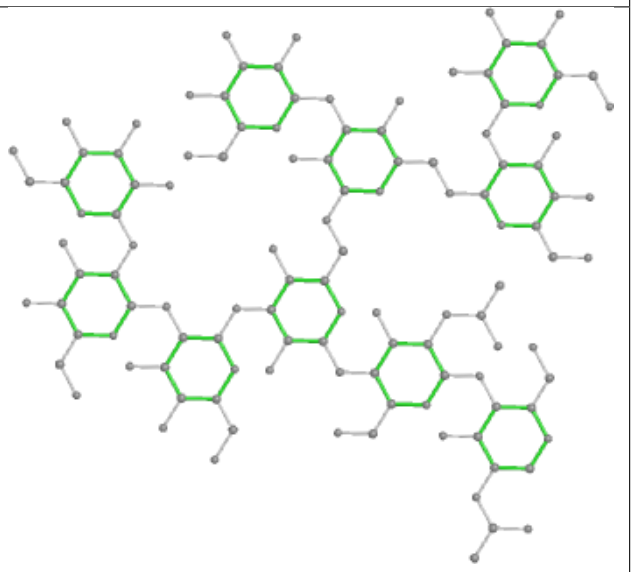
Bond lengths



Bond angles

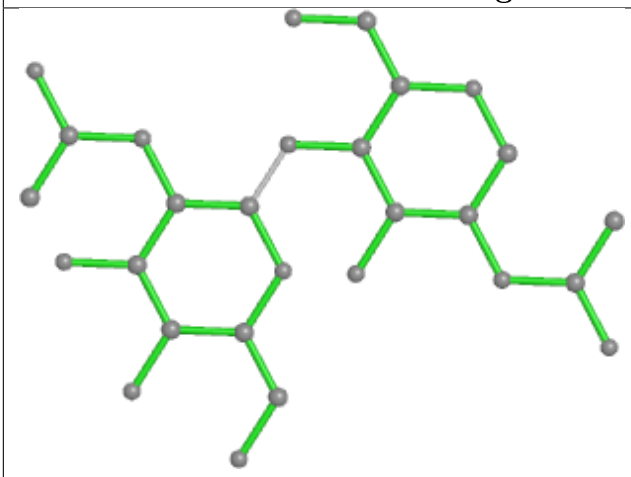


Torsions

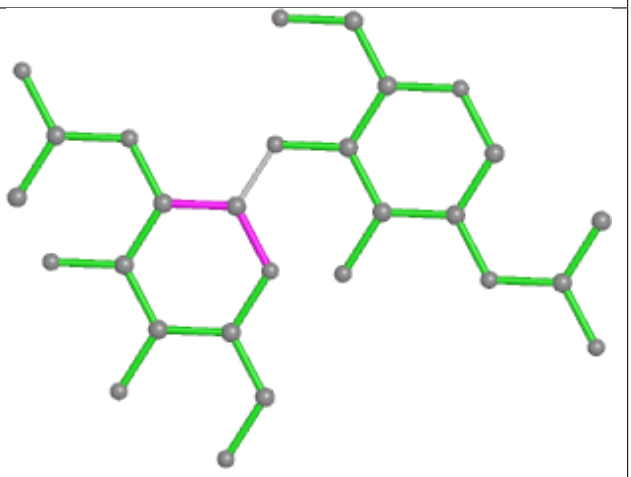


Rings

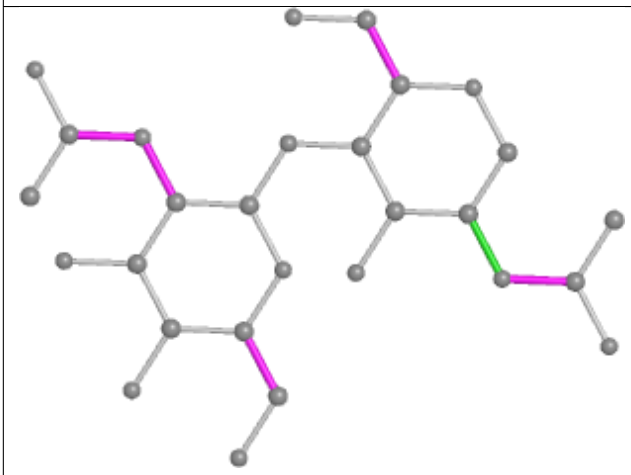
Oligosaccharide Chain T



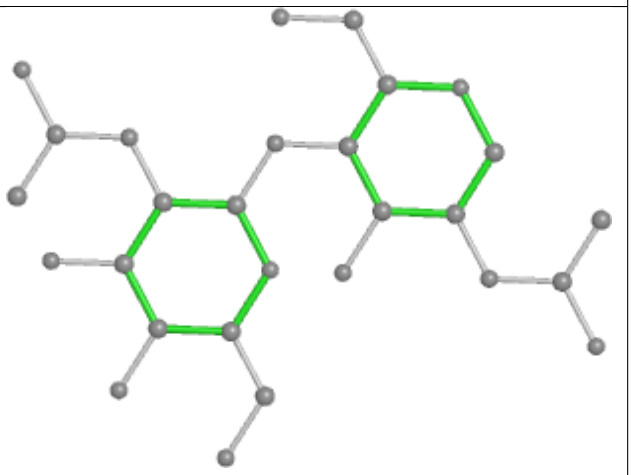
Bond lengths



Bond angles

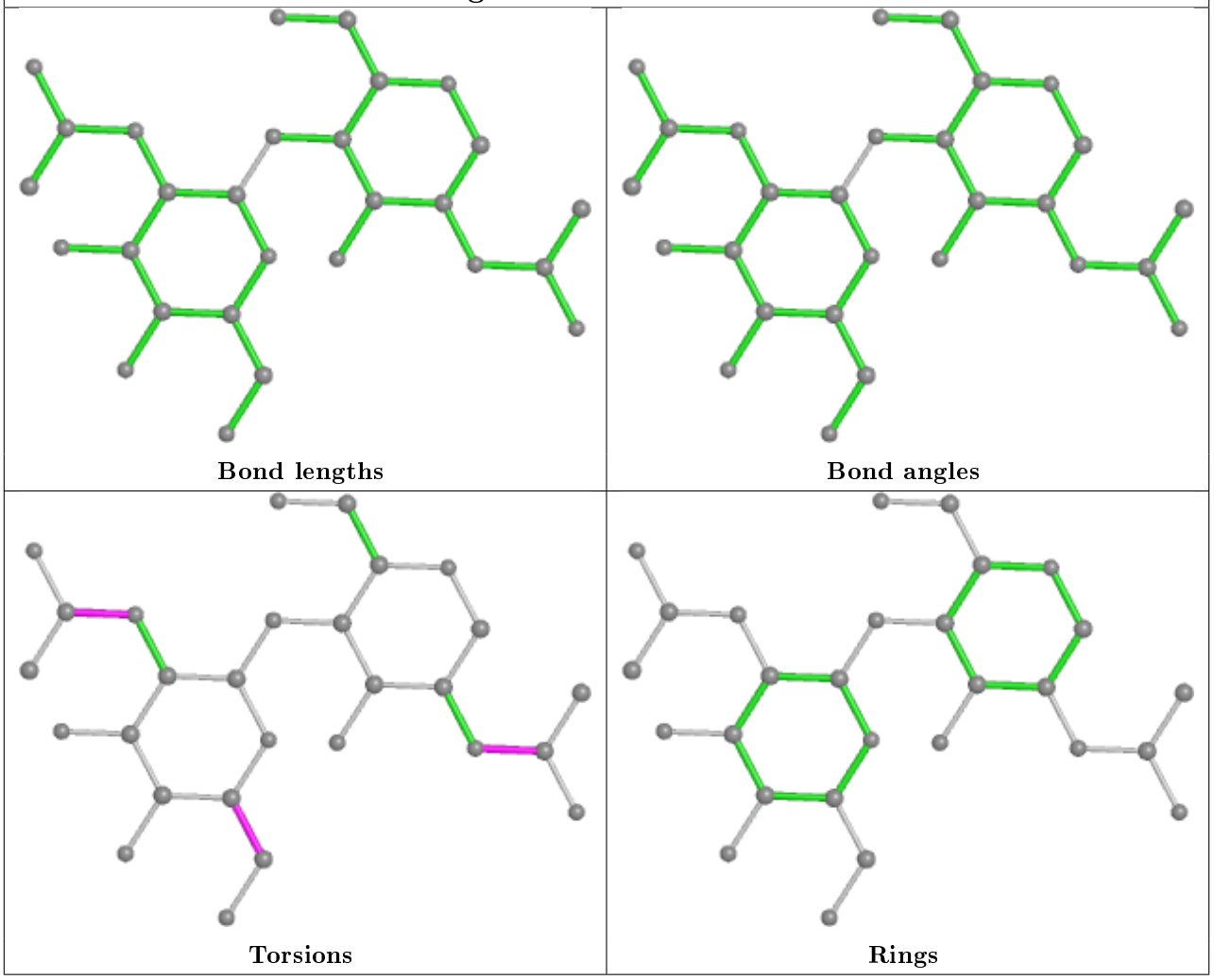


Torsions



Rings

Oligosaccharide Chain U



5.6 Ligand geometry

Of 34 ligands modelled in this entry, 4 are monoatomic - leaving 30 for Mogul analysis.

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	$\#\|Z\| > 2$
9	GOL	N	301	-	5,5,5	0.24	0	5,5,5	0.29	0
7	NAG	O	516	1	14,14,15	0.29	0	17,19,21	0.58	0
7	NAG	K	514	1	14,14,15	0.88	1 (7%)	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	GOL	D	301	-	5,5,5	0.24	0	5,5,5	0.29	0
7	NAG	E	516	1	14,14,15	0.64	0	17,19,21	0.74	0
7	NAG	O	513	1	14,14,15	1.09	2 (14%)	17,19,21	0.90	1 (5%)
7	NAG	A	516	1	14,14,15	0.52	0	17,19,21	0.58	0
7	NAG	O	512	1	14,14,15	0.64	0	17,19,21	0.73	1 (5%)
7	NAG	K	511	1	14,14,15	0.55	0	17,19,21	0.47	0
7	NAG	K	512	1	14,14,15	0.66	0	17,19,21	0.66	0
7	NAG	O	514	1	14,14,15	0.47	0	17,19,21	1.07	1 (5%)
7	NAG	A	517	1	14,14,15	0.61	0	17,19,21	0.78	1 (5%)
7	NAG	K	513	1	14,14,15	0.70	1 (7%)	17,19,21	0.95	1 (5%)
7	NAG	A	519	1	14,14,15	0.46	0	17,19,21	0.61	0
7	NAG	E	512	1	14,14,15	0.28	0	17,19,21	0.87	1 (5%)
7	NAG	E	518	1	14,14,15	0.29	0	17,19,21	0.41	0
7	NAG	A	515	1	14,14,15	0.63	0	17,19,21	0.60	0
7	NAG	O	515	1	14,14,15	1.06	1 (7%)	17,19,21	0.62	0
7	NAG	K	515	1	14,14,15	0.68	1 (7%)	17,19,21	0.75	0
7	NAG	E	517	1	14,14,15	0.34	0	17,19,21	0.46	0
7	NAG	E	513	1	14,14,15	0.65	1 (7%)	17,19,21	0.67	0
7	NAG	E	514	1	14,14,15	0.62	0	17,19,21	1.02	1 (5%)
7	NAG	O	517	1	14,14,15	0.41	0	17,19,21	0.34	0
7	NAG	A	520	1	14,14,15	0.53	0	17,19,21	0.81	1 (5%)
7	NAG	E	515	1	14,14,15	0.85	2 (14%)	17,19,21	0.74	0
9	GOL	J	301	-	5,5,5	0.23	0	5,5,5	0.28	0
7	NAG	E	511	1	14,14,15	1.19	1 (7%)	17,19,21	0.91	1 (5%)
7	NAG	O	511	1	14,14,15	0.20	0	17,19,21	0.81	1 (5%)
7	NAG	A	518	1	14,14,15	0.87	1 (7%)	17,19,21	0.42	0
9	GOL	Q	301	-	5,5,5	0.24	0	5,5,5	0.28	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
9	GOL	N	301	-	-	4/4/4/4	-
7	NAG	O	516	1	-	0/6/23/26	0/1/1/1
7	NAG	K	514	1	-	2/6/23/26	0/1/1/1
9	GOL	D	301	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	E	516	1	-	0/6/23/26	0/1/1/1
7	NAG	O	513	1	-	2/6/23/26	0/1/1/1
7	NAG	A	516	1	-	2/6/23/26	0/1/1/1
7	NAG	O	512	1	-	2/6/23/26	0/1/1/1
7	NAG	K	511	1	-	0/6/23/26	0/1/1/1
7	NAG	K	512	1	-	2/6/23/26	0/1/1/1
7	NAG	O	514	1	-	0/6/23/26	0/1/1/1
7	NAG	A	517	1	-	0/6/23/26	0/1/1/1
7	NAG	K	513	1	-	2/6/23/26	0/1/1/1
7	NAG	A	519	1	-	2/6/23/26	0/1/1/1
7	NAG	E	512	1	-	3/6/23/26	0/1/1/1
7	NAG	E	518	1	-	0/6/23/26	0/1/1/1
7	NAG	A	515	1	-	1/6/23/26	0/1/1/1
7	NAG	O	515	1	-	2/6/23/26	0/1/1/1
7	NAG	K	515	1	-	2/6/23/26	0/1/1/1
7	NAG	E	517	1	-	1/6/23/26	0/1/1/1
7	NAG	E	513	1	-	2/6/23/26	0/1/1/1
7	NAG	E	514	1	-	2/6/23/26	0/1/1/1
7	NAG	O	517	1	-	1/6/23/26	0/1/1/1
7	NAG	A	520	1	-	6/6/23/26	0/1/1/1
7	NAG	E	515	1	-	0/6/23/26	0/1/1/1
9	GOL	J	301	-	-	0/4/4/4	-
7	NAG	E	511	1	-	4/6/23/26	0/1/1/1
7	NAG	O	511	1	-	0/6/23/26	0/1/1/1
7	NAG	A	518	1	-	0/6/23/26	0/1/1/1
9	GOL	Q	301	-	-	4/4/4/4	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	511	NAG	O5-C1	-3.98	1.37	1.43
7	O	515	NAG	O5-C1	-3.68	1.37	1.43
7	O	513	NAG	O5-C1	3.30	1.49	1.43
7	A	518	NAG	O5-C1	-2.86	1.39	1.43
7	K	514	NAG	C1-C2	2.86	1.56	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	513	NAG	C1-O5-C5	3.18	116.50	112.19
7	O	511	NAG	C1-O5-C5	2.75	115.91	112.19
7	O	514	NAG	C1-O5-C5	2.74	115.90	112.19
7	E	512	NAG	C1-O5-C5	2.50	115.58	112.19
7	O	513	NAG	C1-O5-C5	2.44	115.50	112.19

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	N	301	GOL	O1-C1-C2-C3
9	N	301	GOL	C1-C2-C3-O3
9	D	301	GOL	O1-C1-C2-C3
9	D	301	GOL	C1-C2-C3-O3
9	Q	301	GOL	C1-C2-C3-O3

There are no ring outliers.

14 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	301	GOL	3	0
7	O	516	NAG	5	0
7	K	514	NAG	2	0
9	D	301	GOL	5	0
7	E	516	NAG	1	0
7	A	516	NAG	1	0
7	O	512	NAG	1	0
7	K	511	NAG	2	0
7	A	515	NAG	6	0
7	O	515	NAG	5	0
7	E	513	NAG	1	0
7	A	520	NAG	2	0
7	E	515	NAG	1	0
9	J	301	GOL	14	0

5.7 Other polymers (i)

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	302/309 (97%)	0.34	11 (3%) 42 40	34, 62, 99, 136	0
1	E	303/309 (98%)	0.37	20 (6%) 18 18	19, 44, 96, 113	0
1	K	303/309 (98%)	0.43	19 (6%) 20 20	25, 64, 97, 121	0
1	O	303/309 (98%)	0.25	10 (3%) 46 44	23, 46, 82, 111	0
2	B	175/184 (95%)	0.45	9 (5%) 28 26	31, 71, 111, 124	0
2	F	175/184 (95%)	0.71	22 (12%) 3 3	25, 53, 120, 138	0
2	H	176/184 (95%)	0.73	22 (12%) 3 3	36, 83, 124, 133	0
2	L	173/184 (94%)	0.72	18 (10%) 6 6	50, 94, 121, 131	0
3	C	210/214 (98%)	0.19	8 (3%) 40 38	31, 54, 81, 97	0
3	I	210/214 (98%)	-0.14	1 (0%) 91 91	25, 42, 63, 78	0
3	M	210/214 (98%)	-0.11	0 100 100	18, 30, 47, 55	0
3	P	210/214 (98%)	0.02	1 (0%) 91 91	18, 42, 76, 90	0
4	D	225/236 (95%)	0.27	9 (4%) 38 36	28, 54, 101, 115	0
4	J	226/236 (95%)	0.09	1 (0%) 92 93	19, 38, 71, 93	0
4	N	228/236 (96%)	0.11	4 (1%) 68 66	18, 32, 66, 89	0
4	Q	228/236 (96%)	0.09	3 (1%) 77 76	21, 47, 92, 104	0
All	All	3657/3772 (96%)	0.27	158 (4%) 35 33	18, 51, 103, 138	0

The worst 5 of 158 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	107	HIS	7.1
2	L	142	LYS	6.5
2	F	109	LEU	5.4
2	F	108	LEU	5.3
1	A	240	LYS	5.1

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
5	MAN	V	10	11/12	0.74	0.29	68,72,83,83	0
6	NAG	U	2	14/15	0.77	0.34	106,116,124,125	0
5	MAN	G	10	11/12	0.79	0.25	76,79,85,86	0
5	MAN	G	9	11/12	0.81	0.30	52,64,75,77	0
5	MAN	R	9	11/12	0.83	0.35	61,77,86,93	0
5	MAN	R	10	11/12	0.83	0.36	66,71,76,77	0
6	NAG	T	2	14/15	0.84	0.33	65,95,105,112	0
5	MAN	S	10	11/12	0.85	0.34	61,73,82,83	0
6	NAG	U	1	14/15	0.88	0.28	79,89,102,102	0
5	MAN	G	7	11/12	0.89	0.20	56,60,67,70	0
5	MAN	V	7	11/12	0.89	0.21	53,62,69,70	0
5	MAN	V	8	11/12	0.90	0.20	63,66,75,79	0
5	MAN	R	7	11/12	0.91	0.21	51,56,62,63	0
5	MAN	G	8	11/12	0.91	0.16	57,63,70,71	0
5	MAN	G	6	11/12	0.91	0.24	26,32,37,43	0
5	BMA	R	3	11/12	0.91	0.18	35,43,53,56	0
5	MAN	S	9	11/12	0.92	0.27	60,75,83,88	0
5	MAN	V	9	11/12	0.92	0.20	64,77,80,81	0
5	NAG	V	1	14/15	0.93	0.20	33,44,51,56	0
5	MAN	S	7	11/12	0.93	0.18	53,57,68,69	0
5	BMA	V	3	11/12	0.93	0.17	38,46,53,59	0
5	MAN	R	4	11/12	0.94	0.17	38,48,57,62	0
5	NAG	V	2	14/15	0.94	0.19	33,40,46,50	0
5	MAN	S	8	11/12	0.94	0.18	58,70,79,79	0
5	MAN	R	8	11/12	0.94	0.17	67,74,78,81	0
5	BMA	G	3	11/12	0.94	0.19	21,28,44,45	0
5	MAN	V	4	11/12	0.94	0.27	35,40,51,55	0
5	MAN	V	6	11/12	0.95	0.16	38,42,52,55	0
6	NAG	T	1	14/15	0.95	0.22	56,69,74,79	0
5	MAN	V	5	11/12	0.95	0.17	33,39,46,46	0
5	MAN	G	5	11/12	0.95	0.21	20,24,30,31	0
5	NAG	G	1	14/15	0.95	0.18	24,27,34,38	0

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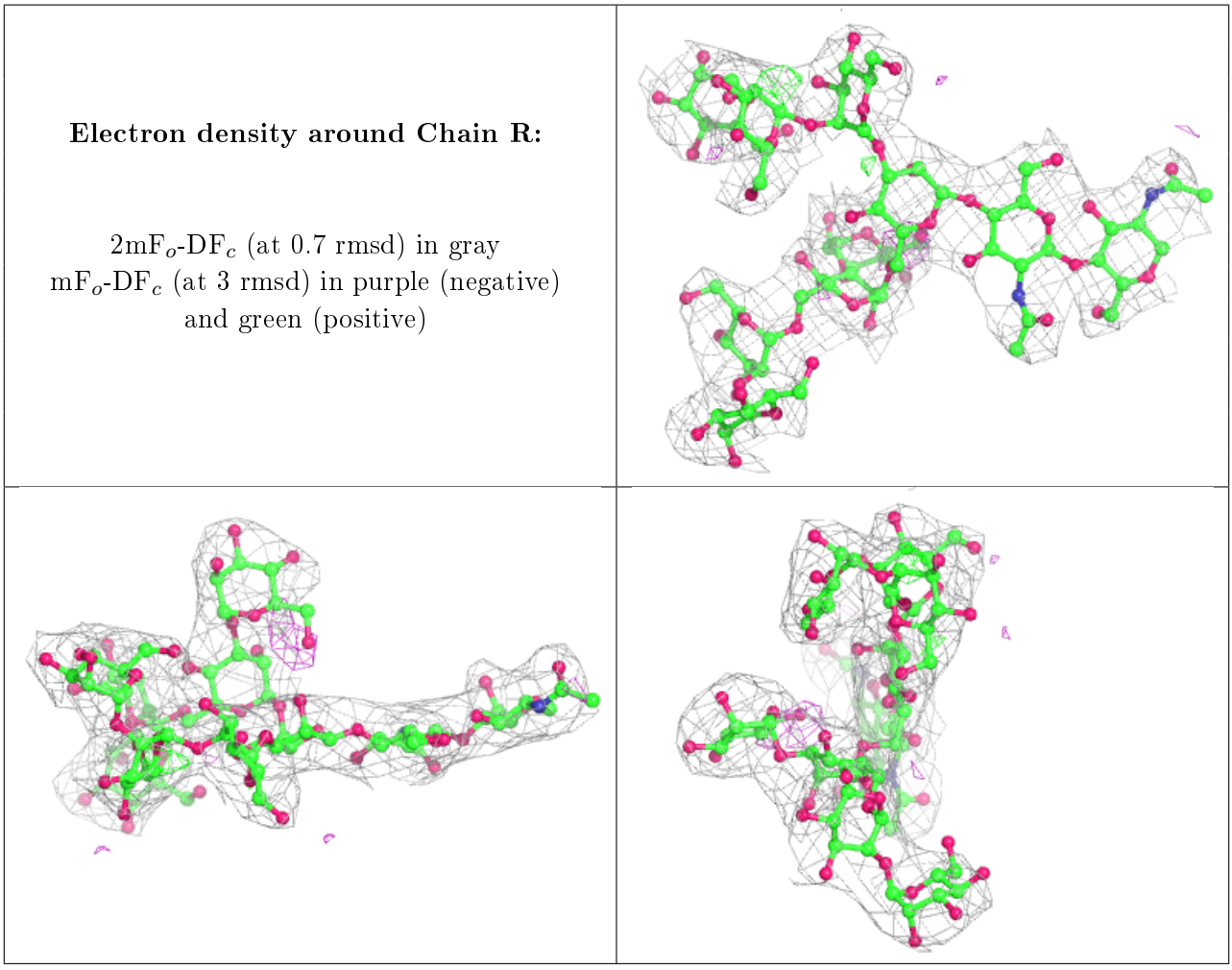
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	S	3	11/12	0.95	0.20	33,38,50,54	0
5	NAG	R	1	14/15	0.96	0.27	30,38,44,44	0
5	MAN	R	5	11/12	0.96	0.17	42,46,51,53	0
5	NAG	R	2	14/15	0.96	0.20	33,38,40,41	0
5	NAG	S	2	14/15	0.96	0.23	30,37,45,47	0
5	MAN	S	6	11/12	0.96	0.18	26,30,36,37	0
5	NAG	S	1	14/15	0.96	0.18	32,40,51,53	0
5	NAG	G	2	14/15	0.96	0.23	25,30,35,37	0
5	MAN	G	4	11/12	0.97	0.18	20,24,30,33	0
5	MAN	R	6	11/12	0.97	0.17	39,42,48,52	0
5	MAN	S	4	11/12	0.98	0.19	24,29,34,41	0
5	MAN	S	5	11/12	0.98	0.20	25,31,40,49	0

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

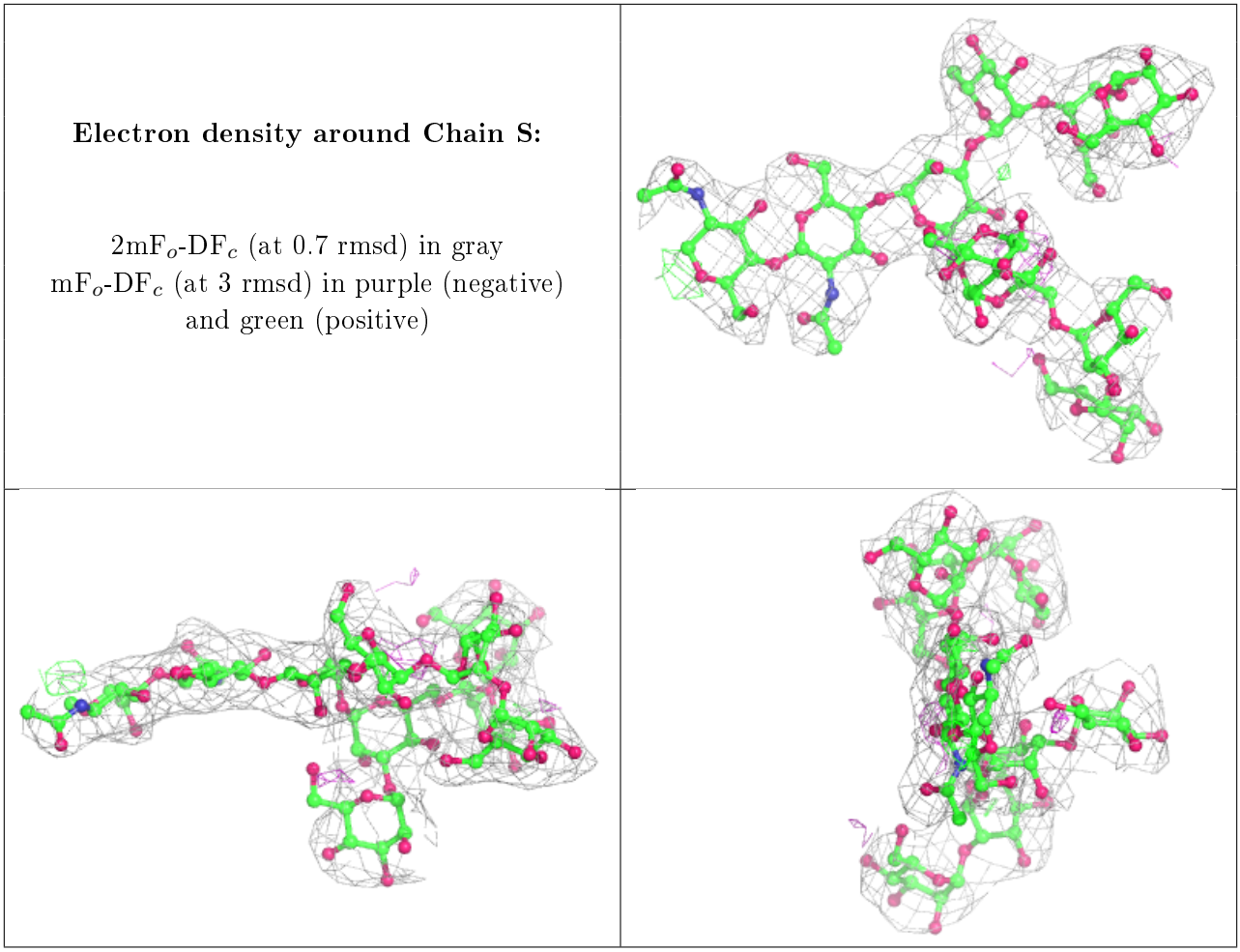
Electron density around Chain R:

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



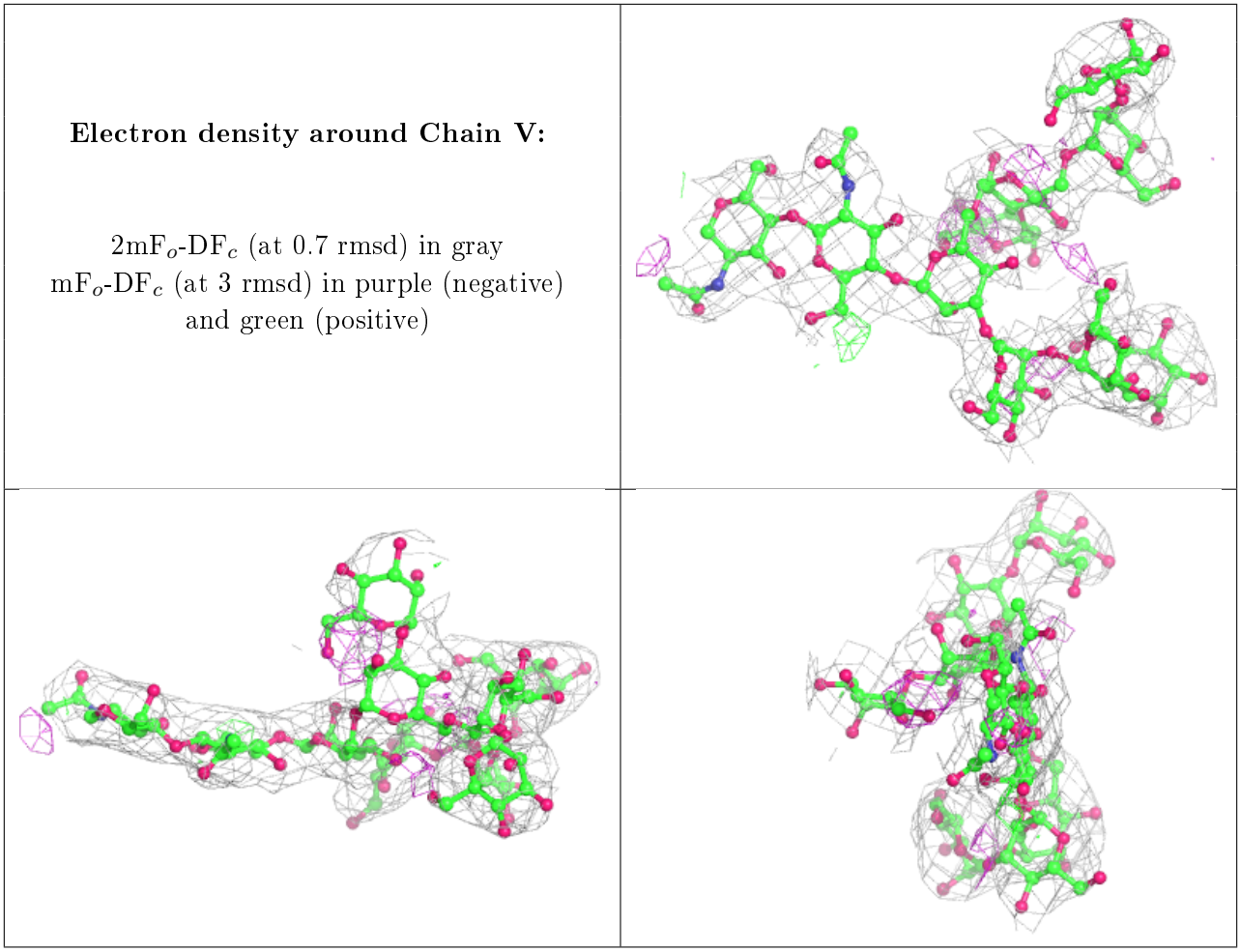
Electron density around Chain S:

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



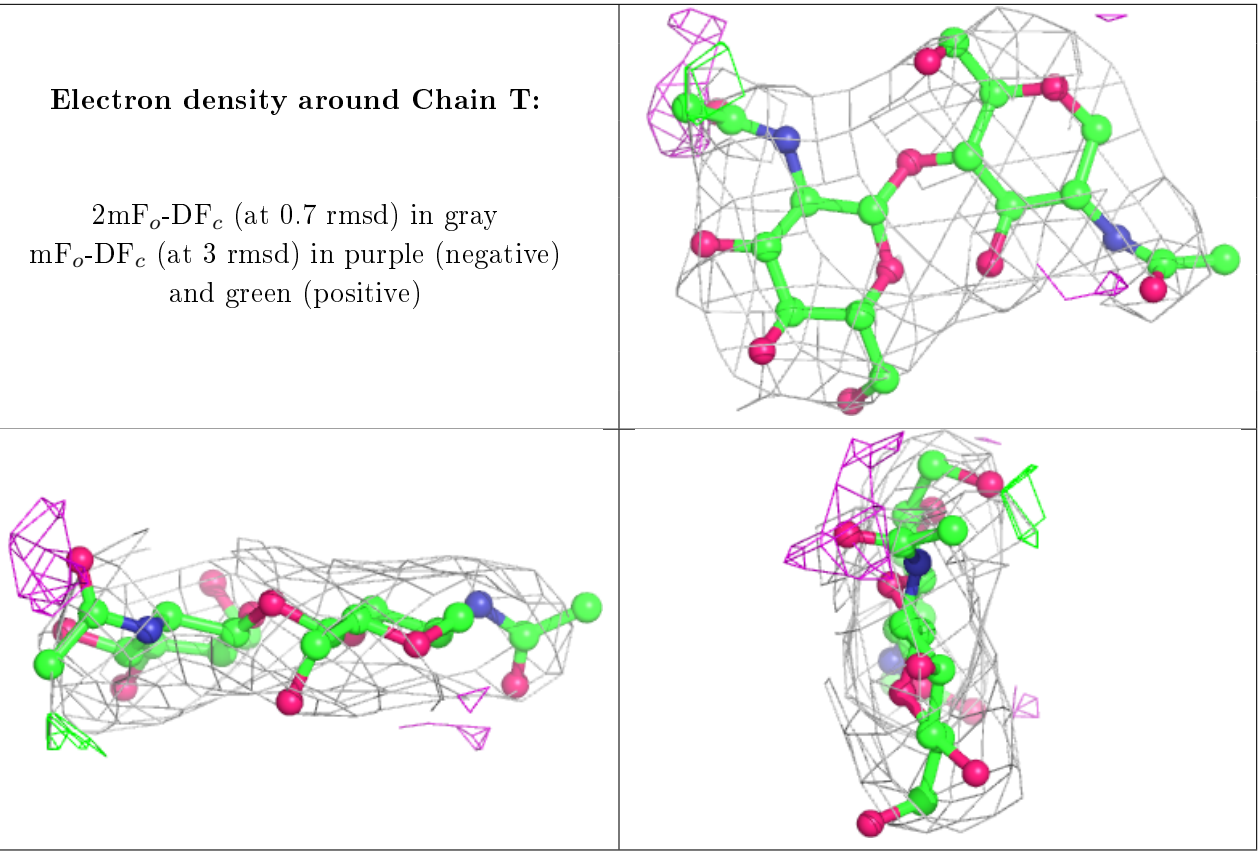
Electron density around Chain V:

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



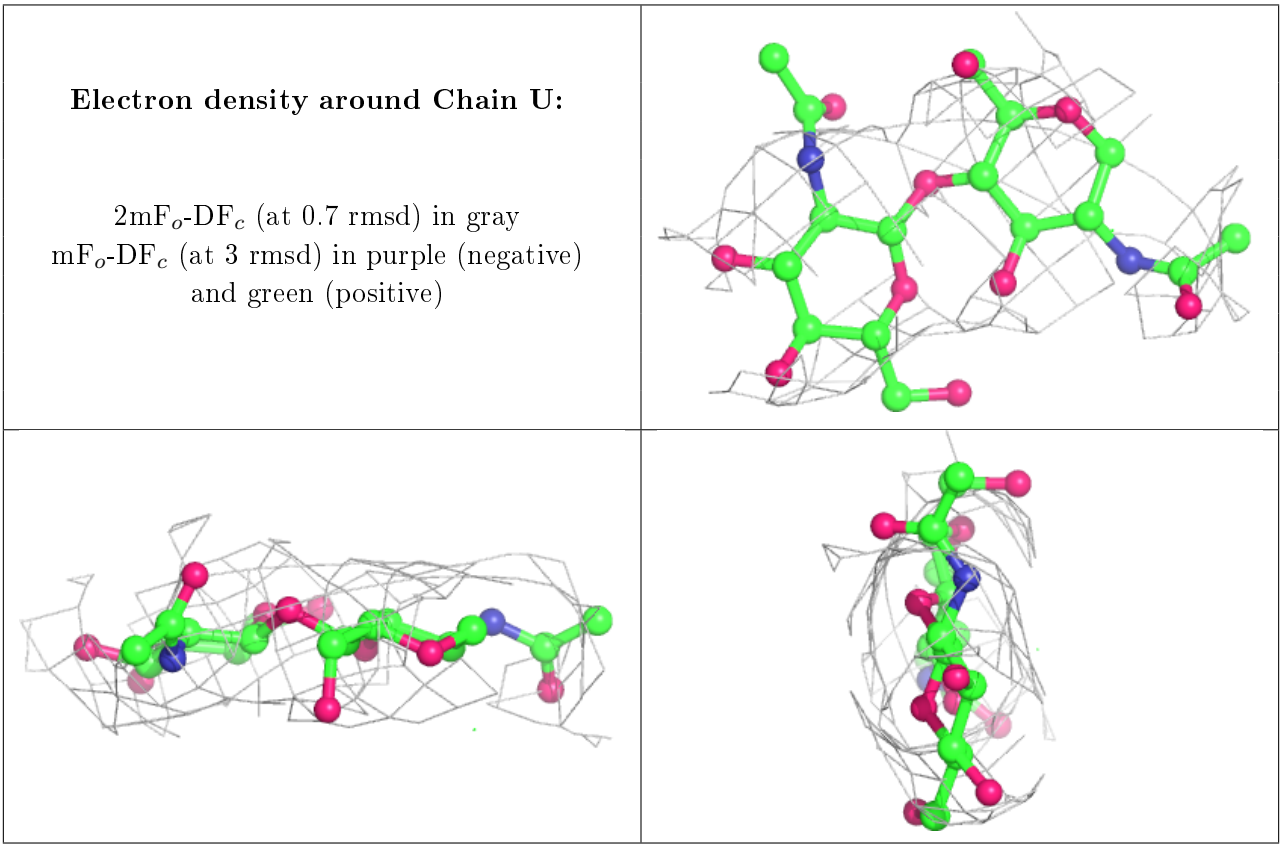
Electron density around Chain T:

$2mF_o$-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 U:

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



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	CL	K	516	1/1	0.39	0.20	70,70,70,70	0
7	NAG	K	514	14/15	0.62	0.35	74,87,92,98	0
8	CL	E	519	1/1	0.67	0.20	53,53,53,53	0
9	GOL	J	301	6/6	0.69	0.29	58,62,66,70	0
9	GOL	D	301	6/6	0.73	0.34	52,55,56,66	0
7	NAG	E	515	14/15	0.76	0.31	44,56,63,63	0
7	NAG	A	517	14/15	0.79	0.40	89,104,113,114	0
8	CL	O	518	1/1	0.80	0.15	54,54,54,54	0
9	GOL	N	301	6/6	0.82	0.23	44,47,53,55	0
7	NAG	A	516	14/15	0.82	0.27	79,96,104,107	0
7	NAG	O	517	14/15	0.83	0.27	69,81,97,99	0
7	NAG	O	514	14/15	0.83	0.27	51,58,67,74	0
7	NAG	E	518	14/15	0.83	0.25	73,82,86,88	0
7	NAG	O	515	14/15	0.84	0.31	49,61,87,87	0
9	GOL	Q	301	6/6	0.84	0.35	48,52,56,59	0
8	CL	A	521	1/1	0.84	0.10	55,55,55,55	0
7	NAG	E	517	14/15	0.85	0.33	52,61,69,70	0
7	NAG	O	516	14/15	0.85	0.41	71,79,83,84	0
7	NAG	E	514	14/15	0.86	0.33	51,56,59,60	0
7	NAG	K	511	14/15	0.86	0.20	78,90,99,100	0
7	NAG	A	519	14/15	0.87	0.31	76,85,90,92	0
7	NAG	K	515	14/15	0.88	0.18	47,64,76,78	0
7	NAG	O	513	14/15	0.88	0.26	48,62,70,78	0
7	NAG	E	516	14/15	0.89	0.33	42,56,65,70	0
7	NAG	A	518	14/15	0.89	0.20	58,62,80,82	0
7	NAG	K	513	14/15	0.89	0.18	65,74,80,91	0
7	NAG	A	515	14/15	0.89	0.26	46,56,64,78	0
7	NAG	O	512	14/15	0.90	0.23	55,63,72,75	0
7	NAG	K	512	14/15	0.90	0.25	53,56,63,74	0
7	NAG	E	512	14/15	0.90	0.21	65,77,88,100	0
7	NAG	E	513	14/15	0.91	0.20	48,55,60,65	0
7	NAG	A	520	14/15	0.91	0.15	63,72,78,83	0
7	NAG	E	511	14/15	0.91	0.26	32,40,50,52	0
7	NAG	O	511	14/15	0.96	0.18	39,43,52,64	0

6.5 Other polymers (i)

There are no such residues in this entry.