Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 08:30 AM EDT

PDB ID	:	5VOD
Title	:	Crystal structure of HCMV Pentamer in complex with neutralizing antibody 9I6
Authors	:	Malito, E.; Chandramouli, S.
Deposited on	:	2017-05-02
Resolution	:	5.90 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

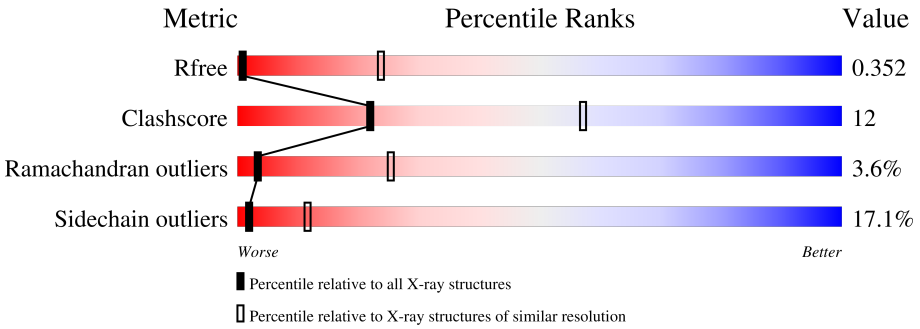
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 5.90 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	1016 (7.94-3.86)
Clashscore	141614	1042 (7.88-3.90)
Ramachandran outliers	138981	1011 (7.94-3.86)
Sidechain outliers	138945	1013 (7.94-3.82)

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

Mol	Chain	Length	Quality of chain
1	A	725	63% 25% • • 8%
2	B	278	63% 21% • 15%
3	C	171	42% 31% • • 23%
4	D	252	45% 16% • 35%
5	E	129	59% 22% • 16%
6	H	288	32% 30% 7% 31%
7	L	241	44% 39% 9% 8%

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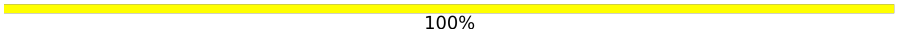
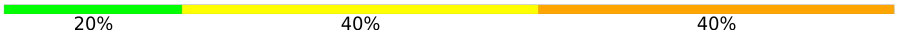
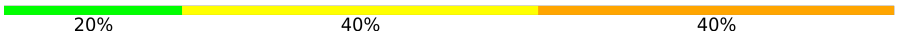
Mol	Chain	Length	Quality of chain
8	F	3	
8	G	3	
8	K	3	
9	I	5	
9	M	5	
10	J	2	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14001 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	667	Total	C	N	O	S	0	0	0
			5358	3427	910	996	25			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	716	GLY	-	expression tag	UNP Q6SW67
A	717	SER	-	expression tag	UNP Q6SW67
A	718	GLY	-	expression tag	UNP Q6SW67
A	719	SER	-	expression tag	UNP Q6SW67
A	720	HIS	-	expression tag	UNP Q6SW67
A	721	HIS	-	expression tag	UNP Q6SW67
A	722	HIS	-	expression tag	UNP Q6SW67
A	723	HIS	-	expression tag	UNP Q6SW67
A	724	HIS	-	expression tag	UNP Q6SW67
A	725	HIS	-	expression tag	UNP Q6SW67

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	237	Total	C	N	O	S	0	0	0
			1867	1188	326	345	8			

- Molecule 3 is a protein called Envelope glycoprotein UL128.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	131	Total	C	N	O	S	0	0	0
			1058	666	190	193	9			

- Molecule 4 is a protein called Envelope glycoprotein UL130.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	164	Total	C	N	O	S	0	0	0
			1337	854	234	241	8			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	215	GLY	-	expression tag	UNP F5HCP3
D	216	SER	-	expression tag	UNP F5HCP3
D	217	GLU	-	expression tag	UNP F5HCP3
D	218	ASN	-	expression tag	UNP F5HCP3
D	219	LEU	-	expression tag	UNP F5HCP3
D	220	TYR	-	expression tag	UNP F5HCP3
D	221	PHE	-	expression tag	UNP F5HCP3
D	222	GLN	-	expression tag	UNP F5HCP3
D	223	ALA	-	expression tag	UNP F5HCP3
D	224	GLY	-	expression tag	UNP F5HCP3
D	225	TRP	-	expression tag	UNP F5HCP3
D	226	SER	-	expression tag	UNP F5HCP3
D	227	HIS	-	expression tag	UNP F5HCP3
D	228	PRO	-	expression tag	UNP F5HCP3
D	229	GLN	-	expression tag	UNP F5HCP3
D	230	PHE	-	expression tag	UNP F5HCP3
D	231	GLU	-	expression tag	UNP F5HCP3
D	232	LYS	-	expression tag	UNP F5HCP3
D	233	GLY	-	expression tag	UNP F5HCP3
D	234	GLY	-	expression tag	UNP F5HCP3
D	235	GLY	-	expression tag	UNP F5HCP3
D	236	SER	-	expression tag	UNP F5HCP3
D	237	GLY	-	expression tag	UNP F5HCP3
D	238	GLY	-	expression tag	UNP F5HCP3
D	239	GLY	-	expression tag	UNP F5HCP3
D	240	SER	-	expression tag	UNP F5HCP3
D	241	GLY	-	expression tag	UNP F5HCP3
D	242	GLY	-	expression tag	UNP F5HCP3
D	243	GLY	-	expression tag	UNP F5HCP3
D	244	SER	-	expression tag	UNP F5HCP3
D	245	TRP	-	expression tag	UNP F5HCP3
D	246	SER	-	expression tag	UNP F5HCP3
D	247	HIS	-	expression tag	UNP F5HCP3
D	248	PRO	-	expression tag	UNP F5HCP3
D	249	GLN	-	expression tag	UNP F5HCP3
D	250	PHE	-	expression tag	UNP F5HCP3
D	251	GLU	-	expression tag	UNP F5HCP3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	252	LYS	-	expression tag	UNP F5HCP3

- Molecule 5 is a protein called Envelope glycoprotein UL131A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	108	Total	C	N	O	S	0	0	0
			893	557	168	166	2			

- Molecule 6 is a protein called Fab 9I6 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	199	Total	C	N	O	S	13	0	0
			1511	965	247	292	7			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	MET	-	initiating methionine	PDB ?
H	246	SER	-	expression tag	UNP S6B291
H	247	SER	-	expression tag	UNP S6B291
H	248	GLY	-	expression tag	UNP S6B291
H	249	LEU	-	expression tag	UNP S6B291
H	250	GLU	-	expression tag	UNP S6B291
H	251	VAL	-	expression tag	UNP S6B291
H	252	LEU	-	expression tag	UNP S6B291
H	253	PHE	-	expression tag	UNP S6B291
H	254	GLN	-	expression tag	UNP S6B291
H	255	GLY	-	expression tag	UNP S6B291
H	256	PRO	-	expression tag	UNP S6B291
H	257	LEU	-	expression tag	UNP S6B291
H	258	GLY	-	expression tag	UNP S6B291
H	259	SER	-	expression tag	UNP S6B291
H	260	ALA	-	expression tag	UNP S6B291
H	261	TRP	-	expression tag	UNP S6B291
H	262	SER	-	expression tag	UNP S6B291
H	263	HIS	-	expression tag	UNP S6B291
H	264	PRO	-	expression tag	UNP S6B291
H	265	GLN	-	expression tag	UNP S6B291
H	266	PHE	-	expression tag	UNP S6B291
H	267	GLU	-	expression tag	UNP S6B291
H	268	LYS	-	expression tag	UNP S6B291
H	269	GLY	-	expression tag	UNP S6B291

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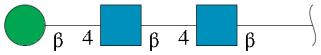
Chain	Residue	Modelled	Actual	Comment	Reference
H	270	GLY	-	expression tag	UNP S6B291
H	271	GLY	-	expression tag	UNP S6B291
H	272	SER	-	expression tag	UNP S6B291
H	273	GLY	-	expression tag	UNP S6B291
H	274	GLY	-	expression tag	UNP S6B291
H	275	GLY	-	expression tag	UNP S6B291
H	276	SER	-	expression tag	UNP S6B291
H	277	GLY	-	expression tag	UNP S6B291
H	278	GLY	-	expression tag	UNP S6B291
H	279	GLY	-	expression tag	UNP S6B291
H	280	SER	-	expression tag	UNP S6B291
H	281	TRP	-	expression tag	UNP S6B291
H	282	SER	-	expression tag	UNP S6B291
H	283	HIS	-	expression tag	UNP S6B291
H	284	PRO	-	expression tag	UNP S6B291
H	285	GLN	-	expression tag	UNP S6B291
H	286	PHE	-	expression tag	UNP S6B291
H	287	GLU	-	expression tag	UNP S6B291
H	288	LYS	-	expression tag	UNP S6B291

- Molecule 7 is a protein called Fab 9I6 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	221	Total	C	N	O	S	53	0	0
			1710	1063	293	345	9			

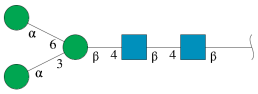
- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 9 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
9	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
9	M	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

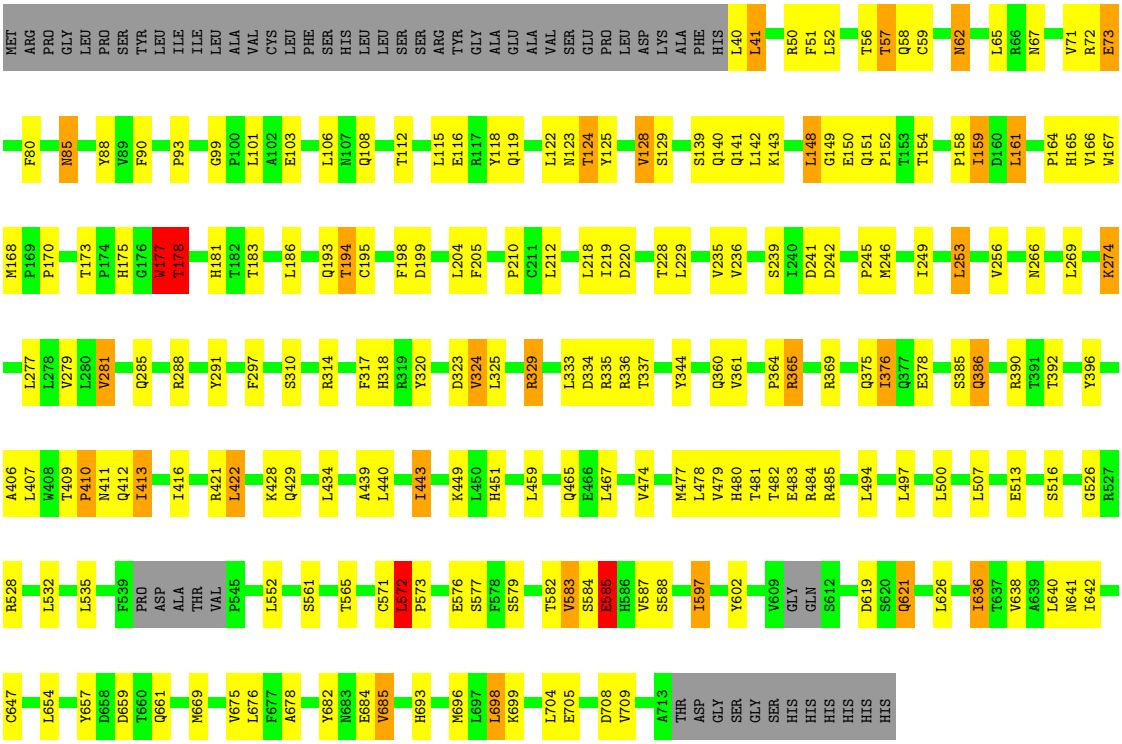
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

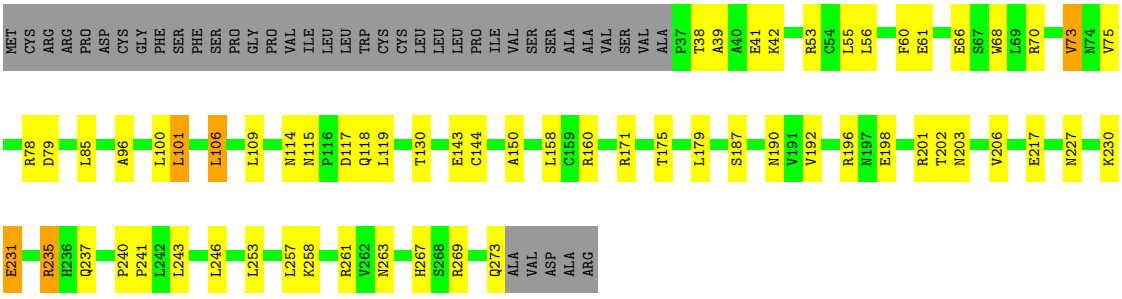
- Molecule 1: Envelope glycoprotein H

Chain A:



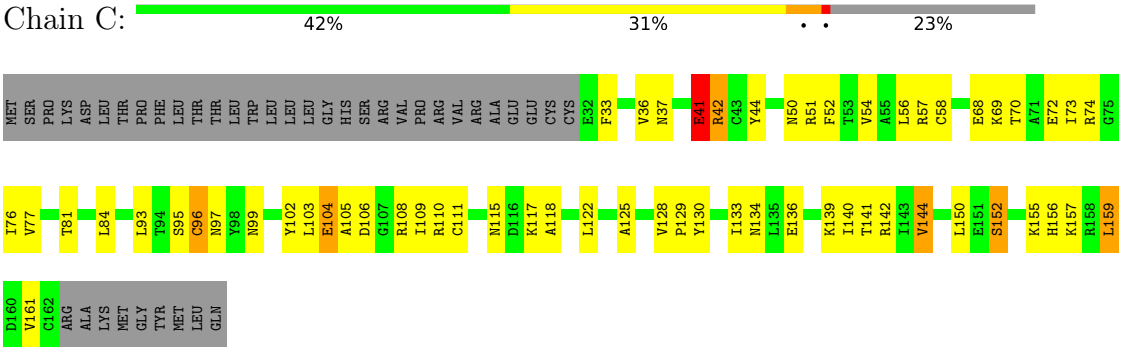
- Molecule 2: Envelope glycoprotein L

Chain B:



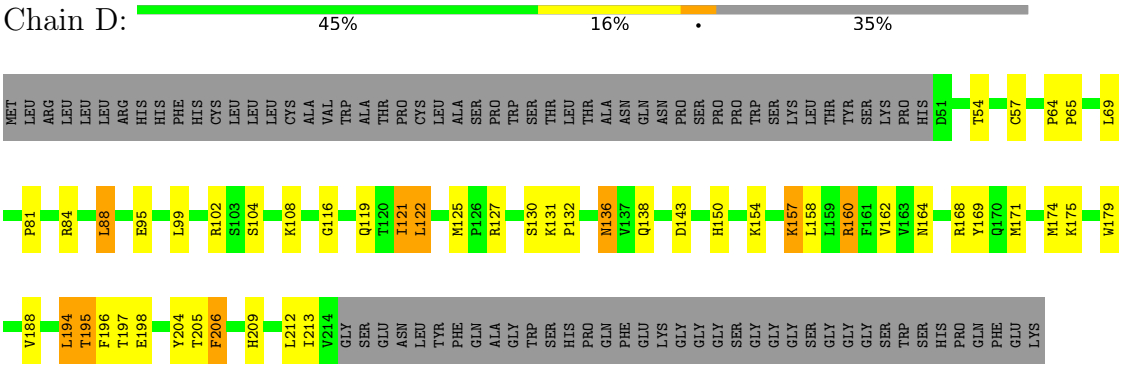
• Molecule 3: Envelope glycoprotein UL128

Chain C:



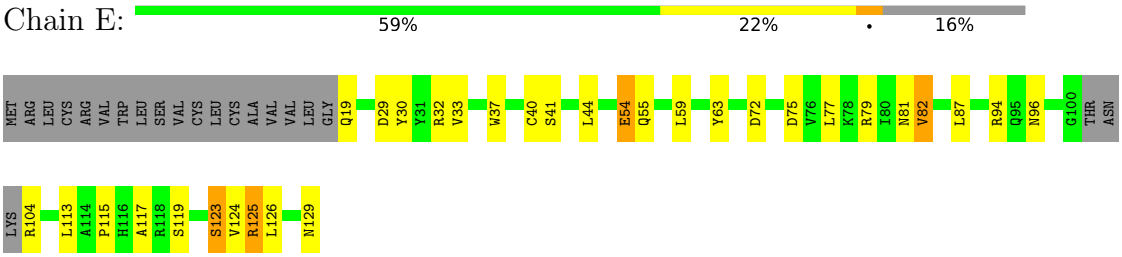
• Molecule 4: Envelope glycoprotein UL130

Chain D:



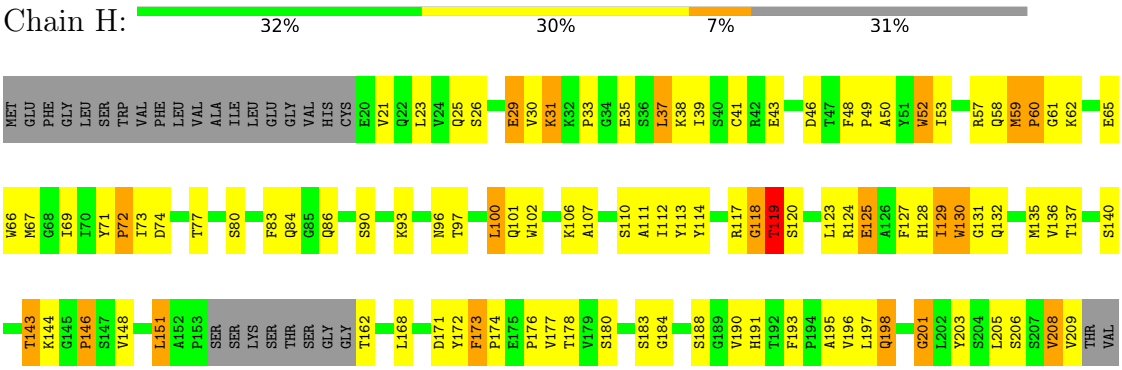
• Molecule 5: Envelope glycoprotein UL131A

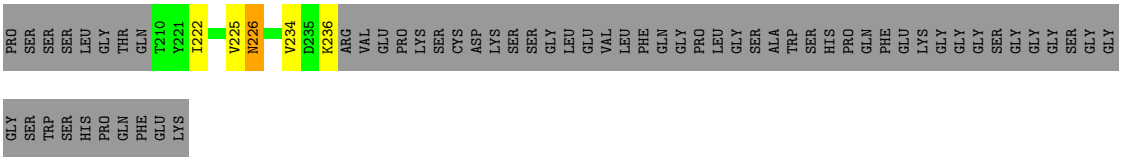
Chain E:



• Molecule 6: Fab 9I6 heavy chain

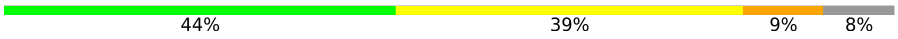
Chain H:

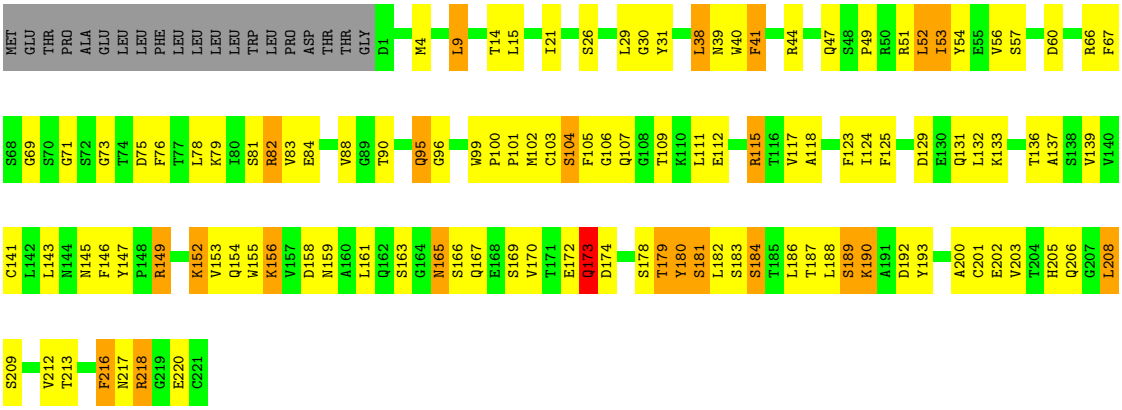




• Molecule 7: Fab 9I6 light chain

Chain L:



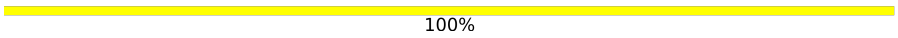


• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

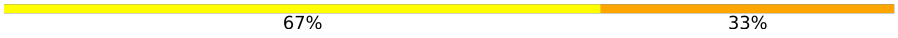
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



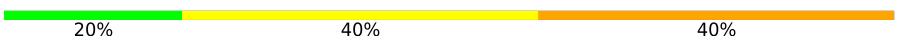
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



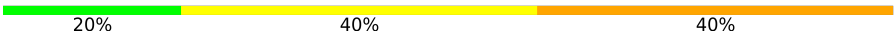
• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 9: 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 M:



• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	148.26Å 208.82Å 267.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.71 – 5.90 89.76 – 5.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.71-5.90) 99.9 (89.76-5.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 5.76Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.258 , 0.299 0.291 , 0.352	Depositor DCC
R_{free} test set	505 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å^2)	276.9	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 264.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	14001	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: MAN, NAG, BMA

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	0.47	0/5484	0.76	1/7473 (0.0%)
2	B	0.53	0/1913	0.74	0/2612
3	C	0.52	0/1080	0.82	0/1461
4	D	0.49	0/1373	0.80	1/1865 (0.1%)
5	E	0.40	0/912	0.63	0/1233
6	H	0.56	0/1550	0.90	0/2112
7	L	0.61	0/1748	0.89	0/2370
All	All	0.51	0/14060	0.79	2/19126 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	136	ASN	C-N-CA	6.59	138.18	121.70
1	A	177	TRP	C-N-CA	5.26	134.86	121.70

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	5358	0	5309	99	1
2	B	1867	0	1859	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1058	0	1050	42	0
4	D	1337	0	1312	28	0
5	E	893	0	851	16	0
6	H	1511	0	1477	69	0
7	L	1710	0	1644	74	0
8	F	39	0	34	1	0
8	G	39	0	34	0	0
8	K	39	0	34	1	0
9	I	61	0	52	2	0
9	M	61	0	52	2	0
10	J	28	0	25	2	0
All	All	14001	0	13733	325	1

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 12.

All (325) 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)
6:H:52:TRP:HA	6:H:71:TYR:CE1	1.84	1.11
6:H:53:ILE:HG12	6:H:72:PRO:HD3	1.27	1.11
6:H:225:VAL:HB	6:H:234:VAL:HB	1.43	0.98
6:H:52:TRP:HA	6:H:71:TYR:HE1	1.16	0.96
3:C:103:LEU:HG	3:C:109:ILE:HG12	1.48	0.95
6:H:195:ALA:HB1	6:H:203:TYR:HB3	1.51	0.93
3:C:74:ARG:HG3	3:C:105:ALA:HA	1.48	0.93
7:L:205:HIS:CG	7:L:206:GLN:H	1.88	0.91
6:H:52:TRP:HB2	6:H:127:PHE:CZ	2.07	0.89
6:H:53:ILE:HG12	6:H:72:PRO:CD	2.03	0.88
7:L:99:TRP:CE3	7:L:101:PRO:HD2	2.08	0.87
7:L:118:ALA:O	7:L:205:HIS:HE1	1.56	0.87
6:H:52:TRP:HB2	6:H:127:PHE:HZ	1.39	0.86
1:A:219:ILE:HG13	1:A:386:GLN:HE21	1.40	0.85
6:H:53:ILE:CG1	6:H:72:PRO:HD3	2.08	0.83
7:L:169:SER:HB3	7:L:183:SER:HB3	1.61	0.82
7:L:131:GLN:HB3	7:L:137:ALA:HA	1.65	0.79
3:C:108:ARG:HD3	5:E:30:TYR:OH	1.84	0.77
1:A:71:VAL:HG11	2:B:179:LEU:HB3	1.67	0.77
2:B:144:CYS:HB3	3:C:144:VAL:HG11	1.66	0.77
6:H:26:SER:OG	6:H:39:ILE:HB	1.85	0.76
1:A:678:ALA:HA	1:A:685:VAL:HG21	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:GLU:HG3	4:D:205:THR:HG21	1.69	0.74
6:H:49:PRO:HB3	6:H:73:ILE:HG12	1.70	0.73
1:A:159:ILE:HD12	1:A:159:ILE:H	1.49	0.73
7:L:115:ARG:HD2	7:L:179:THR:HG23	1.69	0.73
3:C:81:THR:HA	3:C:84:LEU:HD13	1.70	0.72
6:H:52:TRP:CA	6:H:71:TYR:HE1	1.99	0.72
1:A:528:ARG:HH12	1:A:561:SER:HA	1.55	0.72
1:A:584:SER:O	1:A:585:GLU:HB3	1.90	0.72
6:H:113:TYR:HD1	6:H:136:VAL:HG23	1.55	0.71
1:A:482:THR:HG23	1:A:585:GLU:HG3	1.71	0.71
1:A:484:ARG:NH2	1:A:565:THR:HB	2.05	0.71
1:A:219:ILE:HG13	1:A:386:GLN:NE2	2.06	0.70
1:A:194:THR:HA	1:A:210:PRO:HA	1.74	0.70
9:M:1:NAG:H62	9:M:2:NAG:C7	2.21	0.70
4:D:81:PRO:HD3	10:J:1:NAG:H2	1.74	0.70
7:L:123:PHE:HB3	7:L:125:PHE:CE2	2.28	0.69
6:H:86:GLN:O	6:H:106:LYS:NZ	2.21	0.69
3:C:95:SER:O	3:C:96:CYS:HB2	1.92	0.69
6:H:124:ARG:HB3	7:L:99:TRP:HE1	1.59	0.68
6:H:146:PRO:HB3	6:H:172:TYR:HB3	1.76	0.68
1:A:62:ASN:H	2:B:241:PRO:HG3	1.58	0.67
3:C:103:LEU:HD13	3:C:122:LEU:HD23	1.77	0.67
6:H:124:ARG:HB3	7:L:99:TRP:NE1	2.09	0.67
6:H:38:LYS:HG3	6:H:101:GLN:HB3	1.77	0.67
7:L:201:CYS:O	7:L:213:THR:HA	1.95	0.67
7:L:205:HIS:CG	7:L:206:GLN:N	2.63	0.66
3:C:108:ARG:HH22	3:C:110:ARG:HH21	1.43	0.65
7:L:124:ILE:HD13	7:L:201:CYS:HB2	1.78	0.64
1:A:218:LEU:HA	1:A:386:GLN:HB2	1.80	0.64
7:L:118:ALA:O	7:L:205:HIS:CE1	2.45	0.64
3:C:74:ARG:HG3	3:C:105:ALA:CA	2.25	0.64
1:A:181:HIS:CE1	1:A:411:ASN:HB3	2.33	0.63
1:A:407:LEU:HG	1:A:422:LEU:HD11	1.81	0.63
1:A:239:SER:HB2	1:A:245:PRO:HB3	1.81	0.63
6:H:25:GLN:HB2	6:H:132:GLN:HB3	1.81	0.63
6:H:124:ARG:HB3	7:L:99:TRP:CD1	2.33	0.63
6:H:195:ALA:HB1	6:H:203:TYR:CB	2.28	0.62
7:L:57:SER:HB3	7:L:69:GLY:O	1.99	0.62
6:H:197:LEU:HG	6:H:201:GLY:HA2	1.80	0.62
7:L:153:VAL:HA	7:L:202:GLU:O	1.99	0.62
3:C:111:CYS:SG	5:E:32:ARG:HD2	2.39	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:LEU:HD22	3:C:159:LEU:H	1.65	0.62
1:A:485:ARG:HH22	1:A:588:SER:HB3	1.64	0.61
3:C:74:ARG:HD2	3:C:104:GLU:O	2.01	0.60
1:A:159:ILE:H	1:A:159:ILE:CD1	2.13	0.60
3:C:81:THR:HG23	3:C:122:LEU:HD13	1.83	0.60
7:L:136:THR:HB	7:L:187:THR:HG22	1.82	0.60
1:A:166:VAL:HG21	1:A:413:ILE:HG22	1.84	0.60
4:D:206:PHE:HD2	4:D:206:PHE:O	1.83	0.60
3:C:73:ILE:HA	3:C:76:ILE:HD12	1.84	0.60
1:A:205:PHE:HD1	2:B:231:GLU:HG2	1.67	0.59
6:H:113:TYR:CD1	6:H:136:VAL:HG23	2.35	0.59
4:D:54:THR:HA	4:D:57:CYS:SG	2.42	0.59
7:L:9:LEU:O	7:L:109:THR:HA	2.03	0.59
1:A:219:ILE:H	1:A:386:GLN:HE21	1.51	0.59
1:A:602:TYR:HB3	1:A:636:ILE:HG22	1.82	0.59
3:C:69:LYS:HB2	3:C:72:GLU:CG	2.32	0.59
6:H:83:PHE:HA	6:H:86:GLN:HB2	1.84	0.59
1:A:246:MET:HG3	1:A:281:VAL:HG13	1.85	0.59
1:A:583:VAL:HG23	1:A:584:SER:H	1.68	0.59
1:A:344:TYR:HD1	1:A:376:ILE:HG23	1.68	0.59
7:L:38:LEU:HD23	7:L:56:VAL:HG22	1.85	0.58
3:C:103:LEU:CG	3:C:109:ILE:HG12	2.29	0.58
6:H:53:ILE:HD12	6:H:117:ARG:HG3	1.85	0.58
7:L:172:GLU:HA	7:L:180:TYR:CE1	2.38	0.58
7:L:53:ILE:HD13	7:L:78:LEU:HD11	1.85	0.58
7:L:152:LYS:HE3	7:L:154:GLN:HB2	1.86	0.58
7:L:66:ARG:HG2	7:L:82:ARG:HD2	1.86	0.58
7:L:38:LEU:HG	7:L:56:VAL:HA	1.85	0.57
7:L:165:ASN:HB2	7:L:186:LEU:HG	1.86	0.57
1:A:459:LEU:HD21	1:A:467:LEU:HD12	1.86	0.57
1:A:396:TYR:H	1:A:429:GLN:NE2	2.02	0.57
6:H:33:PRO:HD3	6:H:140:SER:HA	1.86	0.57
7:L:41:PHE:CZ	7:L:51:ARG:HA	2.40	0.57
1:A:572:LEU:HD13	1:A:597:ILE:HD13	1.88	0.56
3:C:74:ARG:HH11	3:C:104:GLU:N	2.02	0.56
7:L:193:TYR:CE1	7:L:216:PHE:HZ	2.23	0.56
1:A:128:VAL:HG21	1:A:269:LEU:HA	1.88	0.56
6:H:58:GLN:O	6:H:111:ALA:HB1	2.04	0.56
1:A:71:VAL:HG21	2:B:192:VAL:HG11	1.87	0.56
6:H:29:GLU:HG2	6:H:31:LYS:HE3	1.86	0.55
7:L:136:THR:HA	7:L:189:SER:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:155:TRP:HZ2	7:L:184:SER:O	1.89	0.55
6:H:196:VAL:O	6:H:203:TYR:HA	2.06	0.55
3:C:69:LYS:HB2	3:C:72:GLU:HG2	1.88	0.55
3:C:129:PRO:HB2	4:D:164:ASN:HD22	1.72	0.55
3:C:111:CYS:HB3	5:E:32:ARG:NH1	2.22	0.55
6:H:177:VAL:HB	6:H:205:LEU:HD21	1.89	0.54
4:D:154:LYS:HD3	4:D:179:TRP:NE1	2.22	0.54
6:H:52:TRP:CD1	6:H:118:GLY:HA2	2.43	0.54
6:H:180:SER:HB2	6:H:184:GLY:HA2	1.90	0.54
1:A:177:TRP:HE3	1:A:178:THR:H	1.56	0.54
6:H:23:LEU:HB2	6:H:131:GLY:HA2	1.89	0.54
2:B:198:GLU:O	2:B:201:ARG:HD3	2.08	0.53
7:L:154:GLN:HG2	7:L:161:LEU:HD23	1.89	0.53
6:H:66:TRP:CZ3	7:L:102:MET:HA	2.43	0.53
1:A:396:TYR:H	1:A:429:GLN:HE22	1.56	0.53
1:A:698:LEU:HD21	1:A:704:LEU:HD12	1.90	0.53
2:B:187:SER:HB2	2:B:257:LEU:HD11	1.90	0.53
1:A:246:MET:CG	1:A:281:VAL:HG13	2.38	0.53
7:L:95:GLN:HG2	7:L:96:GLY:N	2.23	0.53
10:J:1:NAG:C1	10:J:2:NAG:H2	2.39	0.53
7:L:67:PHE:HA	7:L:79:LYS:O	2.10	0.52
8:F:2:NAG:H3	8:F:3:BMA:O2	2.10	0.52
2:B:231:GLU:O	2:B:235:ARG:HB2	2.09	0.52
6:H:59:MET:HE2	6:H:60:PRO:HD2	1.92	0.52
1:A:67:ASN:HA	1:A:85:ASN:O	2.10	0.52
1:A:573:PRO:HG2	1:A:576:GLU:HG3	1.91	0.52
6:H:190:VAL:HG12	6:H:209:VAL:HG23	1.92	0.52
4:D:157:LYS:HG3	5:E:63:TYR:OH	2.09	0.52
2:B:73:VAL:HG11	2:B:175:THR:HG22	1.91	0.51
6:H:113:TYR:HE1	6:H:136:VAL:HB	1.75	0.51
7:L:95:GLN:HG2	7:L:96:GLY:H	1.74	0.51
1:A:71:VAL:CG1	2:B:179:LEU:HB3	2.39	0.51
1:A:439:ALA:O	1:A:443:ILE:HG23	2.10	0.51
3:C:133:ILE:HD11	4:D:162:VAL:HG13	1.92	0.51
6:H:58:GLN:HB3	6:H:112:ILE:HB	1.91	0.51
6:H:191:HIS:HB2	6:H:208:VAL:HG23	1.93	0.51
3:C:77:VAL:HG11	3:C:103:LEU:CD2	2.41	0.51
6:H:128:HIS:NE2	7:L:54:TYR:HB2	2.25	0.51
6:H:23:LEU:CB	6:H:131:GLY:HA2	2.41	0.51
2:B:150:ALA:HB1	4:D:64:PRO:HG3	1.93	0.50
2:B:240:PRO:HD2	2:B:243:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:LYS:HB2	3:C:72:GLU:HG3	1.93	0.50
4:D:136:ASN:ND2	4:D:138:GLN:HG3	2.25	0.50
5:E:44:LEU:HD11	5:E:87:LEU:HB3	1.93	0.50
7:L:193:TYR:O	7:L:218:ARG:HG3	2.11	0.50
1:A:526:GLY:O	1:A:579:SER:HA	2.12	0.50
1:A:158:PRO:HD2	1:A:161:LEU:HB2	1.93	0.50
4:D:130:SER:HB2	5:E:54:GLU:HB2	1.94	0.50
7:L:40:TRP:CD2	7:L:78:LEU:HD13	2.47	0.49
5:E:75:ASP:O	5:E:79:ARG:HG3	2.12	0.49
6:H:30:VAL:HA	6:H:137:THR:HB	1.93	0.49
6:H:178:THR:OG1	6:H:226:ASN:HB3	2.12	0.49
1:A:124:THR:HG23	1:A:125:TYR:HD1	1.76	0.49
6:H:48:PHE:N	6:H:49:PRO:CD	2.76	0.49
7:L:193:TYR:HE1	7:L:216:PHE:CZ	2.30	0.49
1:A:485:ARG:HD3	1:A:585:GLU:HA	1.94	0.49
7:L:153:VAL:HG22	7:L:203:VAL:HG22	1.94	0.49
1:A:57:THR:HG23	2:B:60:PHE:HB2	1.94	0.49
1:A:333:LEU:HA	1:A:337:THR:HG21	1.95	0.49
2:B:53:ARG:HA	2:B:56:LEU:HD12	1.94	0.49
3:C:42:ARG:HB2	3:C:44:TYR:OH	2.13	0.49
6:H:151:LEU:HD11	6:H:168:LEU:CB	2.42	0.49
7:L:41:PHE:HA	7:L:52:LEU:HB2	1.95	0.49
1:A:285:GLN:HB2	1:A:288:ARG:HH12	1.77	0.49
1:A:477:MET:CE	1:A:479:VAL:HG23	2.42	0.49
3:C:99:ASN:ND2	5:E:37:TRP:H	2.11	0.48
1:A:682:TYR:C	1:A:684:GLU:H	2.16	0.48
5:E:104:ARG:HH22	5:E:129:ASN:HB3	1.78	0.48
2:B:39:ALA:HB3	2:B:60:PHE:HA	1.94	0.48
1:A:219:ILE:HD12	1:A:220:ASP:H	1.78	0.48
2:B:101:LEU:HD13	3:C:157:LYS:HB3	1.95	0.48
6:H:114:TYR:HB3	6:H:130:TRP:CZ3	2.49	0.48
7:L:4:MET:HB2	7:L:106:GLY:HA2	1.95	0.48
1:A:56:THR:HG23	1:A:72:ARG:NH2	2.29	0.47
3:C:95:SER:O	3:C:96:CYS:CB	2.59	0.47
7:L:129:ASP:O	7:L:133:LYS:HB2	2.13	0.47
4:D:119:GLN:HG3	4:D:122:LEU:HB2	1.96	0.47
3:C:130:TYR:OH	5:E:81:ASN:HA	2.14	0.47
4:D:175:LYS:HB3	4:D:195:THR:HG23	1.96	0.47
1:A:148:LEU:O	1:A:151:GLN:HG2	2.14	0.47
6:H:125:GLU:HB2	7:L:39:ASN:HD21	1.79	0.47
1:A:465:GLN:HA	1:A:516:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:LEU:HD13	3:C:159:LEU:N	2.29	0.47
7:L:9:LEU:H	7:L:9:LEU:HG	1.45	0.47
7:L:99:TRP:CZ3	7:L:103:CYS:HA	2.50	0.47
1:A:279:VAL:HG12	1:A:281:VAL:HG22	1.97	0.47
1:A:334:ASP:H	1:A:337:THR:HB	1.79	0.47
7:L:193:TYR:CE1	7:L:216:PHE:CZ	3.02	0.47
6:H:52:TRP:HA	6:H:71:TYR:CD1	2.45	0.46
7:L:155:TRP:CD1	7:L:186:LEU:HD13	2.50	0.46
1:A:485:ARG:NH2	1:A:588:SER:HB3	2.29	0.46
6:H:130:TRP:CZ3	7:L:49:PRO:HD2	2.51	0.46
6:H:30:VAL:HG22	6:H:137:THR:HB	1.96	0.46
6:H:119:THR:HA	6:H:128:HIS:H	1.79	0.46
7:L:88:VAL:HG13	7:L:111:LEU:O	2.15	0.46
1:A:99:GLY:O	1:A:103:GLU:HG2	2.16	0.46
6:H:100:LEU:HD21	6:H:102:TRP:CH2	2.51	0.46
6:H:113:TYR:CD1	6:H:136:VAL:CG2	2.99	0.46
1:A:269:LEU:HB2	1:A:279:VAL:HG23	1.96	0.46
3:C:74:ARG:CD	3:C:104:GLU:O	2.64	0.46
6:H:113:TYR:CE1	6:H:136:VAL:HB	2.50	0.46
1:A:80:PHE:HB2	1:A:88:TYR:HB2	1.98	0.46
4:D:88:LEU:HD12	4:D:102:ARG:HA	1.98	0.46
4:D:121:ILE:HD13	4:D:188:VAL:HG21	1.97	0.46
6:H:193:PHE:HD2	6:H:206:SER:O	1.99	0.46
1:A:128:VAL:HG12	1:A:266:ASN:C	2.36	0.46
1:A:619:ASP:HB3	1:A:621:GLN:OE1	2.16	0.46
4:D:206:PHE:O	4:D:206:PHE:CD2	2.68	0.46
9:I:3:BMA:H62	9:I:5:MAN:H2	1.67	0.46
7:L:115:ARG:HE	7:L:115:ARG:HB2	1.49	0.46
7:L:66:ARG:HA	7:L:81:SER:HB2	1.97	0.45
7:L:170:VAL:HG13	7:L:181:SER:O	2.17	0.45
1:A:181:HIS:HE1	1:A:411:ASN:HD22	1.62	0.45
1:A:320:TYR:O	1:A:324:VAL:HG13	2.17	0.45
3:C:102:TYR:HE1	3:C:118:ALA:HB3	1.80	0.45
4:D:104:SER:O	4:D:108:LYS:HG3	2.16	0.45
1:A:152:PRO:HB3	1:A:364:PRO:HB3	1.98	0.45
3:C:152:SER:O	3:C:161:VAL:HG11	2.16	0.45
1:A:582:THR:HG22	1:A:582:THR:O	2.17	0.45
2:B:106:LEU:HA	2:B:109:LEU:HD12	1.99	0.45
2:B:253:LEU:HB2	2:B:258:LYS:HE2	1.98	0.45
5:E:123:SER:HB2	5:E:125:ARG:HH21	1.82	0.45
7:L:156:LYS:HD2	7:L:202:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:CYS:SG	1:A:93:PRO:HD3	2.57	0.45
1:A:485:ARG:HH22	1:A:588:SER:CB	2.29	0.45
1:A:80:PHE:HZ	2:B:246:LEU:HD12	1.82	0.45
6:H:30:VAL:HG13	6:H:137:THR:CG2	2.46	0.45
7:L:155:TRP:O	7:L:161:LEU:HA	2.17	0.45
7:L:205:HIS:CD2	7:L:206:GLN:H	2.33	0.45
9:I:3:BMA:O5	9:I:5:MAN:H5	2.17	0.45
1:A:451:HIS:HA	1:A:494:LEU:HD21	1.99	0.44
4:D:121:ILE:HD12	5:E:126:LEU:HD12	1.98	0.44
7:L:188:LEU:HB3	7:L:192:ASP:HB2	1.99	0.44
1:A:365:ARG:O	1:A:369:ARG:HG2	2.16	0.44
1:A:378:GLU:HG3	1:A:428:LYS:HE2	1.99	0.44
1:A:636:ILE:HD11	1:A:705:GLU:HB2	1.98	0.44
1:A:181:HIS:NE2	1:A:411:ASN:HB3	2.32	0.44
1:A:235:VAL:HG22	1:A:249:ILE:HG23	1.99	0.44
1:A:406:ALA:HB1	1:A:413:ILE:HG12	2.00	0.44
1:A:669:MET:HE3	1:A:675:VAL:HA	2.00	0.44
1:A:228:THR:HB	1:A:235:VAL:HB	1.98	0.44
6:H:73:ILE:HG13	6:H:74:ASP:H	1.83	0.44
6:H:83:PHE:CD2	6:H:86:GLN:OE1	2.70	0.44
1:A:142:LEU:HD22	1:A:274:LYS:HG3	1.99	0.44
6:H:37:LEU:HD22	6:H:37:LEU:HA	1.85	0.44
6:H:151:LEU:HD11	6:H:168:LEU:HB2	1.98	0.44
7:L:149:ARG:HD3	7:L:180:TYR:CE1	2.53	0.44
3:C:133:ILE:HD13	4:D:160:ARG:HB3	1.98	0.44
4:D:157:LYS:HE3	5:E:72:ASP:OD1	2.17	0.43
6:H:119:THR:HB	6:H:120:SER:H	1.66	0.43
1:A:40:LEU:HB3	1:A:41:LEU:H	1.62	0.43
3:C:77:VAL:HG11	3:C:103:LEU:HD23	1.98	0.43
7:L:56:VAL:HG13	7:L:71:GLY:HA3	2.00	0.43
7:L:208:LEU:HD22	7:L:212:VAL:HG21	2.00	0.43
1:A:477:MET:HE2	1:A:479:VAL:HG23	2.00	0.43
1:A:73:GLU:HG2	2:B:68:TRP:CD1	2.54	0.43
1:A:128:VAL:HG12	1:A:266:ASN:O	2.19	0.43
1:A:281:VAL:HG12	1:A:285:GLN:HG3	2.00	0.43
7:L:156:LYS:HD3	7:L:200:ALA:HB3	2.00	0.43
7:L:173:GLN:HG3	7:L:180:TYR:CE2	2.53	0.43
1:A:241:ASP:HB2	1:A:288:ARG:HD3	1.99	0.43
6:H:71:TYR:CG	6:H:72:PRO:HD2	2.54	0.43
7:L:53:ILE:HG12	7:L:69:GLY:HA3	2.00	0.43
6:H:31:LYS:HD2	6:H:37:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:174:ASP:H	7:L:178:SER:HA	1.83	0.43
1:A:118:TYR:CZ	1:A:122:LEU:HD11	2.54	0.43
1:A:474:VAL:HG23	1:A:484:ARG:HB3	2.00	0.43
3:C:74:ARG:HD2	3:C:104:GLU:C	2.38	0.43
1:A:291:TYR:HB2	1:A:335:ARG:HG3	2.00	0.43
6:H:41:CYS:O	6:H:97:THR:HA	2.18	0.43
7:L:174:ASP:HB2	7:L:178:SER:H	1.84	0.43
3:C:130:TYR:CD2	5:E:82:VAL:HG13	2.54	0.43
7:L:69:GLY:HA2	7:L:78:LEU:HD12	2.00	0.43
1:A:314:ARG:HA	1:A:318:HIS:HB2	2.01	0.42
9:M:2:NAG:O7	9:M:2:NAG:C3	2.67	0.42
1:A:148:LEU:HD22	1:A:310:SER:HB3	2.01	0.42
1:A:106:LEU:C	1:A:108:GLN:H	2.22	0.42
3:C:68:GLU:HG3	3:C:69:LYS:HG3	2.01	0.42
7:L:102:MET:HG3	7:L:104:SER:H	1.85	0.42
1:A:128:VAL:HG13	2:B:263:ASN:CG	2.40	0.42
3:C:54:VAL:HB	3:C:73:ILE:HD12	2.02	0.42
4:D:174:MET:HG3	4:D:196:PHE:CE1	2.55	0.42
8:K:1:NAG:H61	8:K:2:NAG:C7	2.50	0.42
2:B:115:ASN:O	2:B:118:GLN:HB2	2.20	0.42
3:C:74:ARG:NH1	3:C:104:GLU:O	2.53	0.42
6:H:31:LYS:HD2	6:H:37:LEU:CD2	2.50	0.42
4:D:116:GLY:HA3	4:D:150:HIS:CE1	2.54	0.42
7:L:96:GLY:HA3	7:L:99:TRP:CZ2	2.54	0.42
1:A:164:PRO:HG2	1:A:416:ILE:HG21	2.02	0.41
1:A:409:THR:HA	1:A:410:PRO:HD2	1.93	0.41
3:C:125:ALA:O	4:D:212:LEU:HA	2.19	0.41
4:D:121:ILE:HG22	4:D:143:ASP:HB3	2.00	0.41
1:A:657:TYR:CE2	1:A:693:HIS:HB2	2.55	0.41
4:D:197:THR:HG22	5:E:117:ALA:HB2	2.01	0.41
1:A:266:ASN:HD21	2:B:261:ARG:HA	1.85	0.41
1:A:317:PHE:CE2	1:A:376:ILE:HG13	2.56	0.41
1:A:638:VAL:HA	1:A:705:GLU:HB3	2.02	0.41
1:A:253:LEU:HB3	1:A:256:VAL:HB	2.02	0.41
2:B:55:LEU:HD21	2:B:240:PRO:HB3	2.03	0.41
7:L:40:TRP:HB2	7:L:53:ILE:HB	2.03	0.41
7:L:217:ASN:HB3	7:L:220:GLU:HB2	2.01	0.41
6:H:57:ARG:HB2	6:H:67:MET:SD	2.60	0.41
3:C:41:GLU:HB3	3:C:42:ARG:H	1.60	0.41
6:H:129:ILE:HA	7:L:51:ARG:NH1	2.35	0.41
7:L:132:LEU:HD21	7:L:193:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:GLU:HA	2:B:68:TRP:CZ3	2.55	0.41
2:B:96:ALA:O	3:C:159:LEU:HG	2.21	0.41
4:D:64:PRO:HA	4:D:65:PRO:HD3	1.96	0.41
4:D:174:MET:SD	4:D:194:LEU:HD11	2.60	0.41
6:H:30:VAL:HG22	6:H:137:THR:CB	2.51	0.41
7:L:115:ARG:HG2	7:L:178:SER:O	2.20	0.40
1:A:329:ARG:HD2	1:A:336:ARG:NH1	2.36	0.40
7:L:118:ALA:HB3	7:L:147:TYR:H	1.85	0.40
7:L:143:LEU:HD13	7:L:182:LEU:HB3	2.03	0.40
1:A:572:LEU:HD13	1:A:572:LEU:HA	1.92	0.40
4:D:204:TYR:CE1	5:E:115:PRO:HB3	2.57	0.40
1:A:480:HIS:CD2	1:A:480:HIS:N	2.89	0.40
2:B:227:ASN:O	2:B:231:GLU:HB2	2.22	0.40
1:A:90:PHE:HE2	2:B:241:PRO:HG2	1.86	0.40
2:B:187:SER:HA	2:B:253:LEU:HD22	2.03	0.40
6:H:144:LYS:HB3	6:H:173:PHE:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:TRP:NE1	1:A:483:GLU:OE2[8_534]	1.81	0.39

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	661/725 (91%)	598 (90%)	47 (7%)	16 (2%)	6 33
2	B	235/278 (84%)	214 (91%)	19 (8%)	2 (1%)	17 56
3	C	129/171 (75%)	107 (83%)	14 (11%)	8 (6%)	1 16
4	D	162/252 (64%)	155 (96%)	6 (4%)	1 (1%)	25 65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	E	104/129 (81%)	100 (96%)	4 (4%)	0	100 100
6	H	193/288 (67%)	138 (72%)	35 (18%)	20 (10%)	0 8
7	L	219/241 (91%)	161 (74%)	43 (20%)	15 (7%)	1 15
All	All	1703/2084 (82%)	1473 (86%)	168 (10%)	62 (4%)	3 25

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	PRO
1	A	297	PHE
3	C	41	GLU
6	H	46	ASP
6	H	118	GLY
6	H	129	ILE
6	H	171	ASP
6	H	174	PRO
6	H	222	ILE
7	L	83	VAL
7	L	218	ARG
1	A	178	THR
1	A	413	ILE
1	A	583	VAL
2	B	267	HIS
3	C	96	CYS
3	C	97	ASN
3	C	117	LYS
4	D	132	PRO
6	H	60	PRO
6	H	62	LYS
7	L	47	GLN
1	A	173	THR
3	C	136	GLU
6	H	31	LYS
6	H	35	GLU
6	H	72	PRO
7	L	30	GLY
7	L	104	SER
7	L	149	ARG
7	L	173	GLN
7	L	180	TYR
1	A	140	GLN

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Mol	Chain	Res	Type
1	A	412	GLN
1	A	585	GLU
1	A	661	GLN
2	B	38	THR
3	C	134	ASN
3	C	141	THR
3	C	142	ARG
6	H	50	ALA
6	H	107	ALA
6	H	198	GLN
6	H	201	GLY
7	L	100	PRO
7	L	159	ASN
7	L	189	SER
1	A	149	GLY
1	A	572	LEU
6	H	119	THR
6	H	143	THR
7	L	145	ASN
7	L	190	LYS
1	A	62	ASN
1	A	199	ASP
1	A	253	LEU
6	H	146	PRO
1	A	410	PRO
7	L	117	VAL
6	H	61	GLY
7	L	73	GLY
6	H	176	PRO

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	607/655 (93%)	512 (84%)	95 (16%)	2 14
2	B	204/238 (86%)	172 (84%)	32 (16%)	2 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	118/154 (77%)	93 (79%)	25 (21%)	1 6
4	D	150/222 (68%)	129 (86%)	21 (14%)	3 17
5	E	95/114 (83%)	78 (82%)	17 (18%)	2 10
6	H	168/238 (71%)	136 (81%)	32 (19%)	1 8
7	L	195/213 (92%)	154 (79%)	41 (21%)	1 6
All	All	1537/1834 (84%)	1274 (83%)	263 (17%)	2 11

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	50	ARG
1	A	51	PHE
1	A	52	LEU
1	A	57	THR
1	A	58	GLN
1	A	65	LEU
1	A	73	GLU
1	A	85	ASN
1	A	101	LEU
1	A	112	THR
1	A	115	LEU
1	A	116	GLU
1	A	119	GLN
1	A	123	ASN
1	A	124	THR
1	A	128	VAL
1	A	129	SER
1	A	139	SER
1	A	141	GLN
1	A	143	LYS
1	A	148	LEU
1	A	150	GLU
1	A	154	THR
1	A	159	ILE
1	A	161	LEU
1	A	165	HIS
1	A	168	MET
1	A	175	HIS
1	A	177	TRP

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Mol	Chain	Res	Type
1	A	178	THR
1	A	183	THR
1	A	186	LEU
1	A	193	GLN
1	A	194	THR
1	A	195	CYS
1	A	198	PHE
1	A	204	LEU
1	A	212	LEU
1	A	229	LEU
1	A	236	VAL
1	A	242	ASP
1	A	274	LYS
1	A	277	LEU
1	A	281	VAL
1	A	323	ASP
1	A	324	VAL
1	A	325	LEU
1	A	329	ARG
1	A	360	GLN
1	A	361	VAL
1	A	365	ARG
1	A	375	GLN
1	A	376	ILE
1	A	385	SER
1	A	386	GLN
1	A	390	ARG
1	A	392	THR
1	A	421	ARG
1	A	422	LEU
1	A	434	LEU
1	A	440	LEU
1	A	443	ILE
1	A	449	LYS
1	A	478	LEU
1	A	481	THR
1	A	497	LEU
1	A	500	LEU
1	A	507	LEU
1	A	513	GLU
1	A	532	LEU
1	A	535	LEU

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Mol	Chain	Res	Type
1	A	552	LEU
1	A	571	CYS
1	A	572	LEU
1	A	577	SER
1	A	585	GLU
1	A	587	VAL
1	A	597	ILE
1	A	621	GLN
1	A	626	LEU
1	A	636	ILE
1	A	640	LEU
1	A	641	ASN
1	A	642	ILE
1	A	647	CYS
1	A	654	LEU
1	A	659	ASP
1	A	676	LEU
1	A	685	VAL
1	A	696	MET
1	A	698	LEU
1	A	699	LYS
1	A	708	ASP
1	A	709	VAL
2	B	41	GLU
2	B	42	LYS
2	B	61	GLU
2	B	70	ARG
2	B	73	VAL
2	B	75	VAL
2	B	78	ARG
2	B	79	ASP
2	B	85	LEU
2	B	100	LEU
2	B	101	LEU
2	B	106	LEU
2	B	114	ASN
2	B	117	ASP
2	B	119	LEU
2	B	130	THR
2	B	143	GLU
2	B	158	LEU
2	B	160	ARG

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Mol	Chain	Res	Type
2	B	171	ARG
2	B	190	ASN
2	B	196	ARG
2	B	202	THR
2	B	203	ASN
2	B	206	VAL
2	B	217	GLU
2	B	230	LYS
2	B	231	GLU
2	B	235	ARG
2	B	237	GLN
2	B	269	ARG
2	B	273	GLN
3	C	33	PHE
3	C	36	VAL
3	C	37	ASN
3	C	41	GLU
3	C	42	ARG
3	C	50	ASN
3	C	51	ARG
3	C	52	PHE
3	C	56	LEU
3	C	57	ARG
3	C	58	CYS
3	C	70	THR
3	C	93	LEU
3	C	104	GLU
3	C	106	ASP
3	C	115	ASN
3	C	128	VAL
3	C	139	LYS
3	C	140	ILE
3	C	144	VAL
3	C	150	LEU
3	C	152	SER
3	C	155	LYS
3	C	156	HIS
3	C	159	LEU
4	D	69	LEU
4	D	84	ARG
4	D	88	LEU
4	D	95	GLU

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Mol	Chain	Res	Type
4	D	99	LEU
4	D	121	ILE
4	D	122	LEU
4	D	125	MET
4	D	127	ARG
4	D	131	LYS
4	D	157	LYS
4	D	158	LEU
4	D	160	ARG
4	D	168	ARG
4	D	169	TYR
4	D	171	MET
4	D	194	LEU
4	D	195	THR
4	D	206	PHE
4	D	209	HIS
4	D	213	ILE
5	E	19	GLN
5	E	29	ASP
5	E	33	VAL
5	E	40	CYS
5	E	41	SER
5	E	54	GLU
5	E	55	GLN
5	E	59	LEU
5	E	77	LEU
5	E	82	VAL
5	E	94	ARG
5	E	96	ASN
5	E	113	LEU
5	E	119	SER
5	E	123	SER
5	E	124	VAL
5	E	125	ARG
6	H	21	VAL
6	H	29	GLU
6	H	37	LEU
6	H	43	GLU
6	H	52	TRP
6	H	59	MET
6	H	65	GLU
6	H	69	ILE

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Mol	Chain	Res	Type
6	H	77	THR
6	H	80	SER
6	H	84	GLN
6	H	90	SER
6	H	93	LYS
6	H	96	ASN
6	H	100	LEU
6	H	110	SER
6	H	119	THR
6	H	123	LEU
6	H	125	GLU
6	H	130	TRP
6	H	135	MET
6	H	143	THR
6	H	148	VAL
6	H	151	LEU
6	H	162	THR
6	H	173	PHE
6	H	183	SER
6	H	188	SER
6	H	198	GLN
6	H	208	VAL
6	H	226	ASN
6	H	236	LYS
7	L	9	LEU
7	L	14	THR
7	L	15	LEU
7	L	21	ILE
7	L	26	SER
7	L	29	LEU
7	L	31	TYR
7	L	38	LEU
7	L	41	PHE
7	L	44	ARG
7	L	52	LEU
7	L	53	ILE
7	L	60	ASP
7	L	75	ASP
7	L	76	PHE
7	L	82	ARG
7	L	84	GLU
7	L	90	THR

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Mol	Chain	Res	Type
7	L	95	GLN
7	L	105	PHE
7	L	107	GLN
7	L	112	GLU
7	L	115	ARG
7	L	139	VAL
7	L	141	CYS
7	L	146	PHE
7	L	152	LYS
7	L	156	LYS
7	L	158	ASP
7	L	163	SER
7	L	165	ASN
7	L	166	SER
7	L	167	GLN
7	L	173	GLN
7	L	179	THR
7	L	181	SER
7	L	184	SER
7	L	190	LYS
7	L	208	LEU
7	L	209	SER
7	L	216	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	104	GLN
1	A	145	GLN
1	A	151	GLN
1	A	181	HIS
1	A	252	HIS
1	A	271	GLN
1	A	289	HIS
1	A	315	ASN
1	A	331	GLN
1	A	386	GLN
1	A	429	GLN
1	A	480	HIS
1	A	512	HIS
3	C	82	HIS

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Mol	Chain	Res	Type
3	C	99	ASN
4	D	123	GLN
4	D	136	ASN
4	D	164	ASN
4	D	211	ASN
5	E	69	HIS
6	H	198	GLN
6	H	224	ASN
7	L	42	GLN
7	L	98	HIS
7	L	167	GLN
7	L	205	HIS

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)

21 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	$\#\|Z\| > 2$
8	NAG	F	1	8,1	14,14,15	0.60	0	17,19,21	1.59	3 (17%)
8	NAG	F	2	8	14,14,15	0.46	0	17,19,21	0.90	1 (5%)
8	BMA	F	3	8	11,11,12	0.71	0	15,15,17	1.28	2 (13%)
8	NAG	G	1	8,1	14,14,15	0.53	0	17,19,21	1.28	2 (11%)
8	NAG	G	2	8	14,14,15	0.64	0	17,19,21	1.76	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	BMA	G	3	8	11,11,12	0.57	0	15,15,17	0.79	1 (6%)
9	NAG	I	1	9,1	14,14,15	0.31	0	17,19,21	0.77	0
9	NAG	I	2	9	14,14,15	0.54	0	17,19,21	2.77	6 (35%)
9	BMA	I	3	9	11,11,12	0.49	0	15,15,17	1.00	1 (6%)
9	MAN	I	4	9	11,11,12	0.62	0	15,15,17	1.44	1 (6%)
9	MAN	I	5	9	11,11,12	0.58	0	15,15,17	1.27	2 (13%)
10	NAG	J	1	4,10	14,14,15	0.65	0	17,19,21	1.57	4 (23%)
10	NAG	J	2	10	14,14,15	0.74	0	17,19,21	1.47	2 (11%)
8	NAG	K	1	4,8	14,14,15	0.35	0	17,19,21	1.64	2 (11%)
8	NAG	K	2	8	14,14,15	0.39	0	17,19,21	0.97	0
8	BMA	K	3	8	11,11,12	0.56	0	15,15,17	1.26	2 (13%)
9	NAG	M	1	9,5	14,14,15	0.29	0	17,19,21	1.31	2 (11%)
9	NAG	M	2	9	14,14,15	0.26	0	17,19,21	1.13	2 (11%)
9	BMA	M	3	9	11,11,12	0.49	0	15,15,17	1.20	2 (13%)
9	MAN	M	4	9	11,11,12	0.42	0	15,15,17	0.85	0
9	MAN	M	5	9	11,11,12	0.57	0	15,15,17	1.90	1 (6%)

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
8	NAG	F	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	F	2	8	-	3/6/23/26	0/1/1/1
8	BMA	F	3	8	-	1/2/19/22	0/1/1/1
8	NAG	G	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	G	2	8	-	0/6/23/26	0/1/1/1
8	BMA	G	3	8	-	2/2/19/22	0/1/1/1
9	NAG	I	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	I	2	9	-	1/6/23/26	0/1/1/1
9	BMA	I	3	9	-	1/2/19/22	0/1/1/1
9	MAN	I	4	9	-	1/2/19/22	0/1/1/1
9	MAN	I	5	9	-	1/2/19/22	0/1/1/1
10	NAG	J	1	4,10	-	3/6/23/26	0/1/1/1
10	NAG	J	2	10	-	1/6/23/26	0/1/1/1
8	NAG	K	1	4,8	-	0/6/23/26	0/1/1/1
8	NAG	K	2	8	-	2/6/23/26	0/1/1/1
8	BMA	K	3	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	M	1	9,5	-	0/6/23/26	0/1/1/1
9	NAG	M	2	9	-	2/6/23/26	0/1/1/1
9	BMA	M	3	9	-	1/2/19/22	0/1/1/1
9	MAN	M	4	9	-	0/2/19/22	0/1/1/1
9	MAN	M	5	9	-	1/2/19/22	1/1/1/1

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	5	MAN	C1-O5-C5	6.85	121.47	112.19
9	I	2	NAG	O5-C1-C2	-6.67	100.75	111.29
9	I	2	NAG	C1-C2-N2	5.72	120.26	110.49
8	K	1	NAG	O5-C1-C2	-5.37	102.81	111.29
10	J	2	NAG	C1-O5-C5	5.15	119.17	112.19
9	I	4	MAN	C1-O5-C5	4.86	118.78	112.19
8	G	2	NAG	C1-O5-C5	4.43	118.19	112.19
8	F	1	NAG	C3-C4-C5	4.41	118.10	110.24
9	I	2	NAG	C2-N2-C7	4.32	129.05	122.90
9	I	2	NAG	C3-C4-C5	4.11	117.58	110.24
9	M	1	NAG	C1-O5-C5	3.98	117.58	112.19
8	G	2	NAG	O5-C1-C2	3.85	117.36	111.29
10	J	1	NAG	O4-C4-C5	3.82	118.78	109.30
8	G	1	NAG	C1-O5-C5	3.80	117.34	112.19
8	K	3	BMA	C1-O5-C5	3.74	117.26	112.19
9	I	5	MAN	C1-O5-C5	3.27	116.62	112.19
8	K	1	NAG	C1-O5-C5	3.22	116.56	112.19
9	I	5	MAN	C1-C2-C3	3.07	113.44	109.67
8	G	1	NAG	C2-N2-C7	3.06	127.26	122.90
9	M	3	BMA	C1-C2-C3	-3.06	105.91	109.67
8	F	3	BMA	C1-C2-C3	3.04	113.41	109.67
9	I	2	NAG	C1-O5-C5	3.01	116.27	112.19
8	F	2	NAG	C1-O5-C5	2.97	116.22	112.19
10	J	1	NAG	C1-O5-C5	-2.84	108.35	112.19
9	M	2	NAG	C2-N2-C7	2.75	126.82	122.90
8	F	1	NAG	C1-O5-C5	-2.69	108.54	112.19
8	F	1	NAG	C4-C3-C2	2.60	114.83	111.02
8	F	3	BMA	C1-O5-C5	2.58	115.68	112.19
9	M	1	NAG	O5-C1-C2	-2.54	107.27	111.29
8	K	3	BMA	C1-C2-C3	2.47	112.70	109.67
8	G	2	NAG	C1-C2-N2	2.40	114.58	110.49
10	J	1	NAG	C2-N2-C7	2.36	126.26	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	3	BMA	C1-O5-C5	-2.33	109.03	112.19
9	M	2	NAG	C1-C2-N2	2.32	114.44	110.49
9	I	3	BMA	O3-C3-C4	2.26	115.57	110.35
10	J	2	NAG	C2-N2-C7	2.24	126.09	122.90
8	G	3	BMA	C1-O5-C5	2.24	115.22	112.19
9	I	2	NAG	C4-C3-C2	2.10	114.10	111.02
10	J	1	NAG	O4-C4-C3	-2.03	105.66	110.35

There are no chirality outliers.

All (21) torsion outliers are listed below:

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

All (1) ring outliers are listed below:

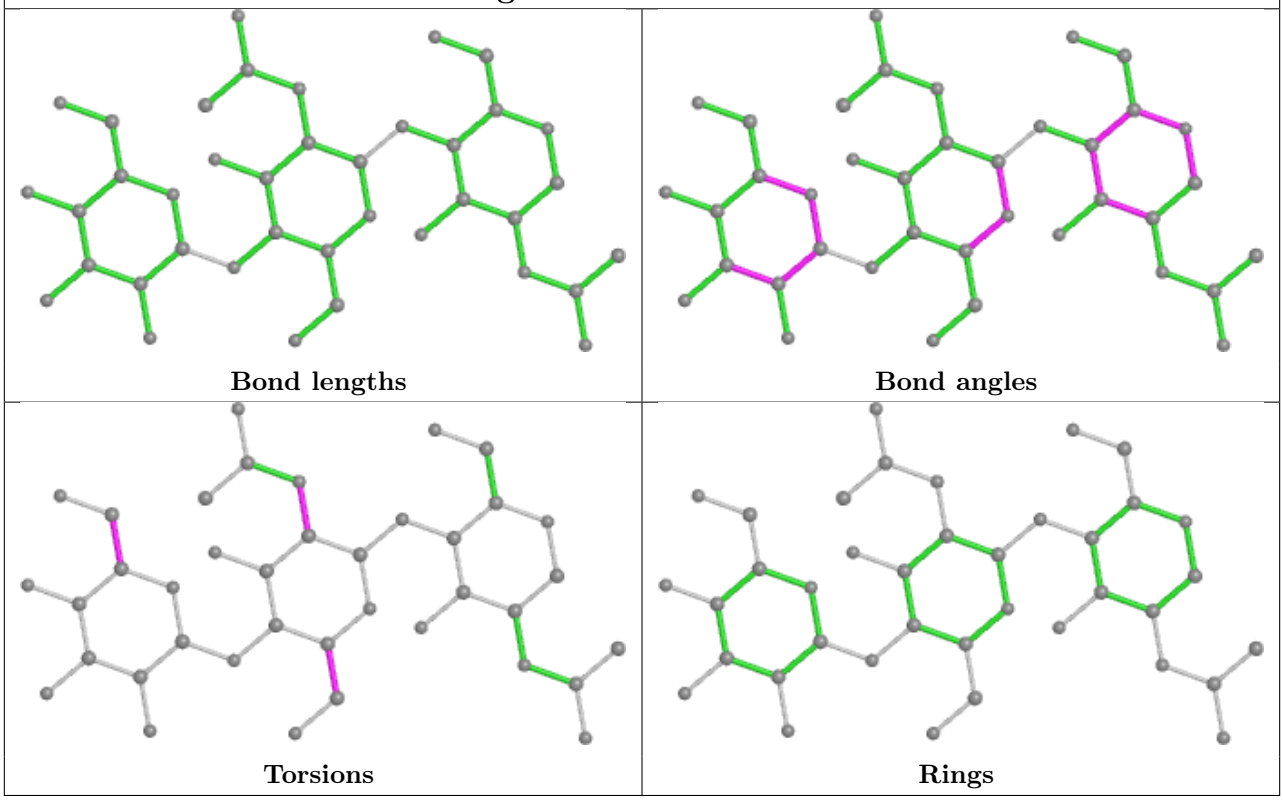
Mol	Chain	Res	Type	Atoms
9	M	5	MAN	C1-C2-C3-C4-C5-O5

10 monomers are involved in 8 short contacts:

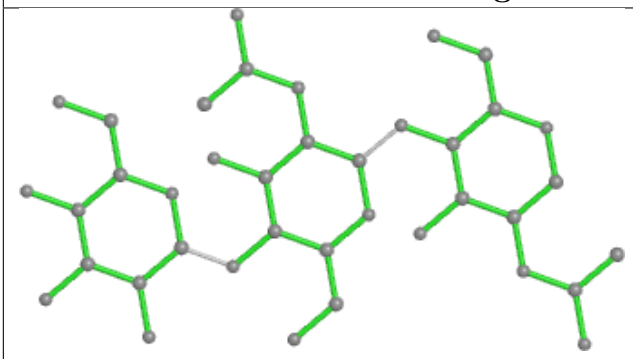
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	2	NAG	2	0
8	F	3	BMA	1	0
8	K	2	NAG	1	0
9	I	3	BMA	2	0
10	J	1	NAG	2	0
10	J	2	NAG	1	0
8	F	2	NAG	1	0
8	K	1	NAG	1	0
9	I	5	MAN	2	0
9	M	1	NAG	1	0

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

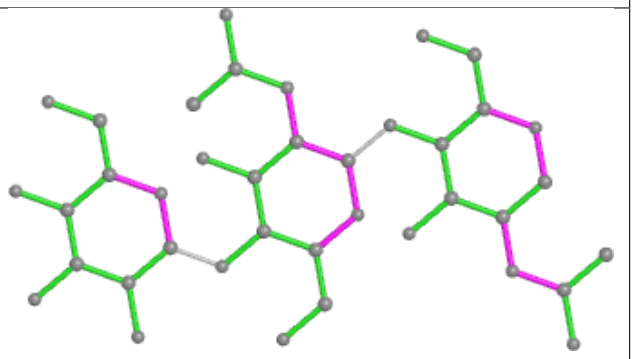
Oligosaccharide Chain F



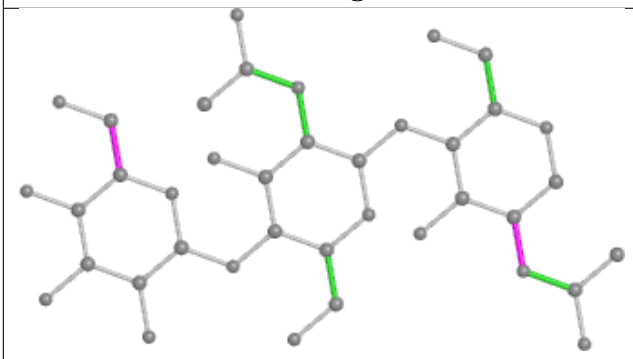
Oligosaccharide Chain G



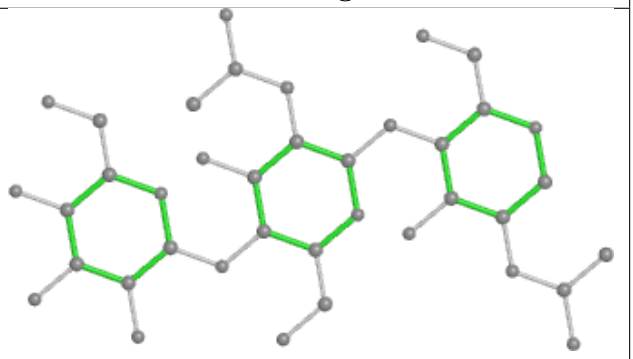
Bond lengths



Bond angles

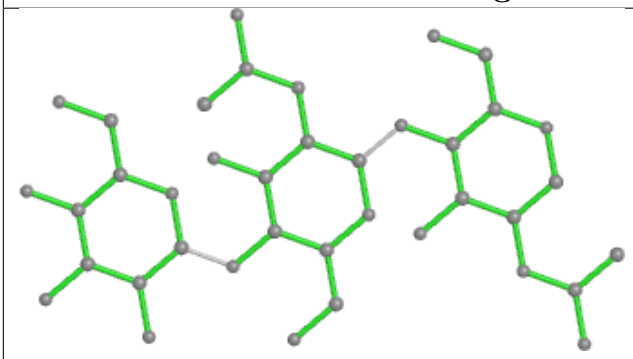


Torsions

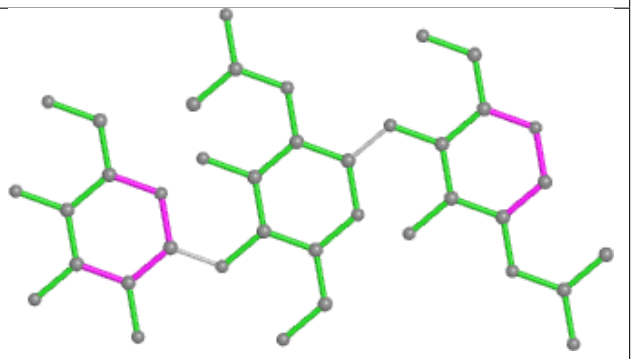


Rings

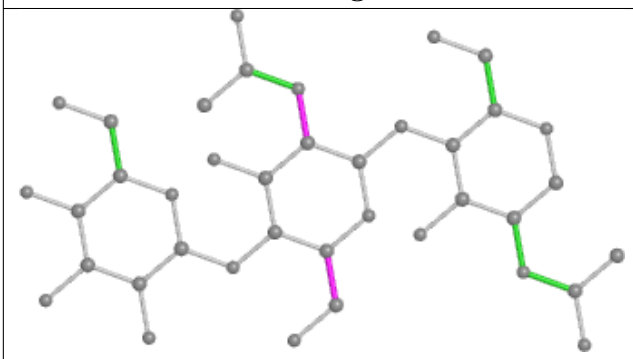
Oligosaccharide Chain K



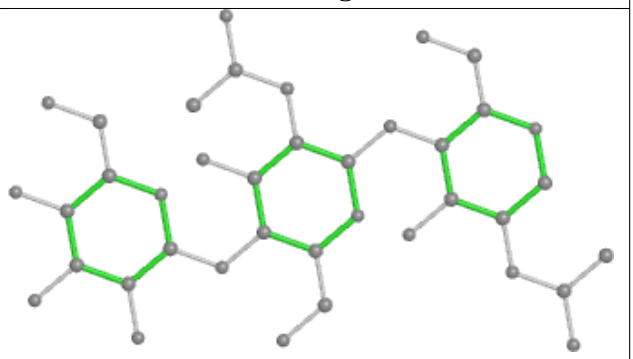
Bond lengths



Bond angles

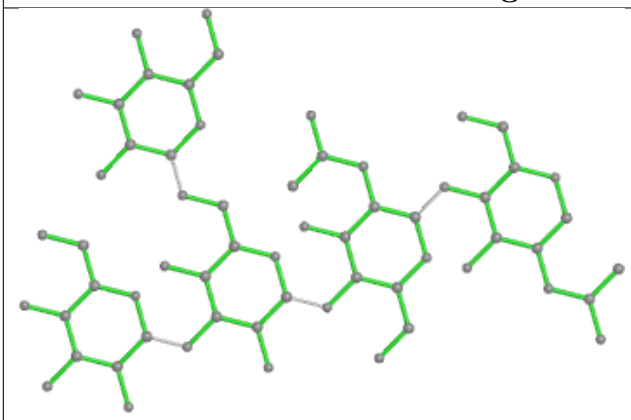


Torsions

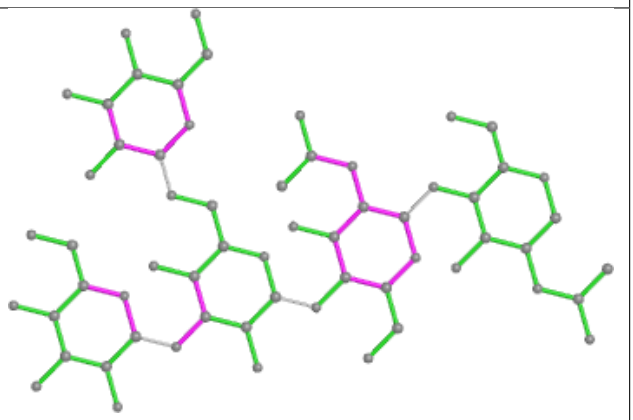


Rings

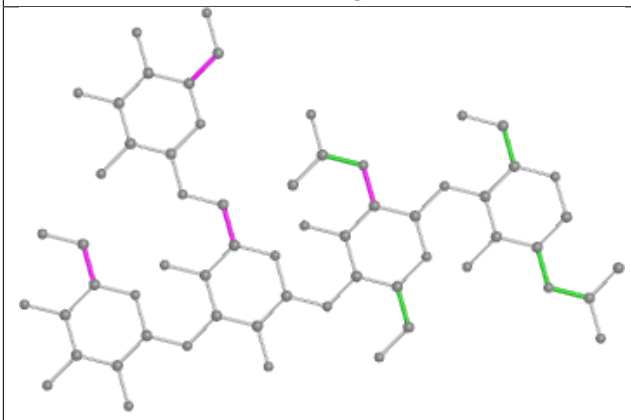
Oligosaccharide Chain I



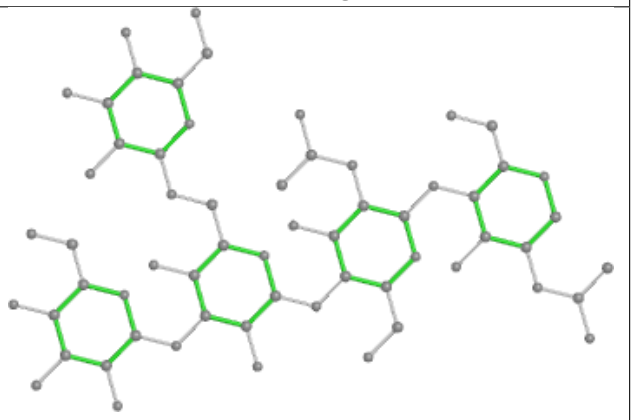
Bond lengths



Bond angles

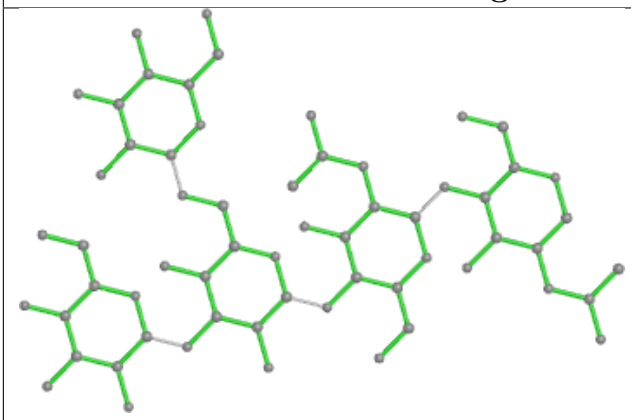


Torsions

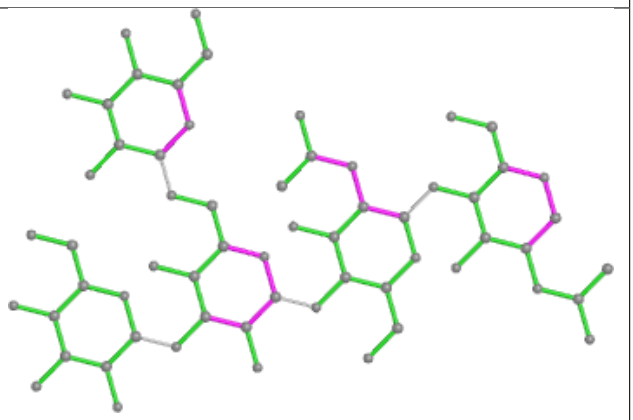


Rings

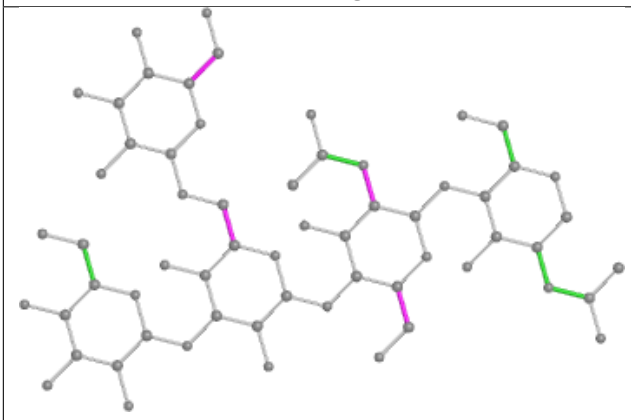
Oligosaccharide Chain M



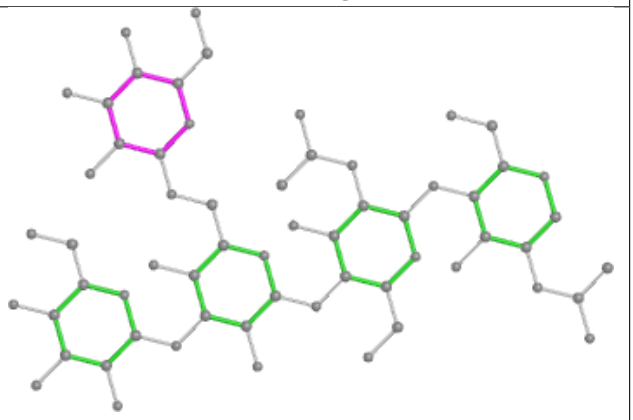
Bond lengths



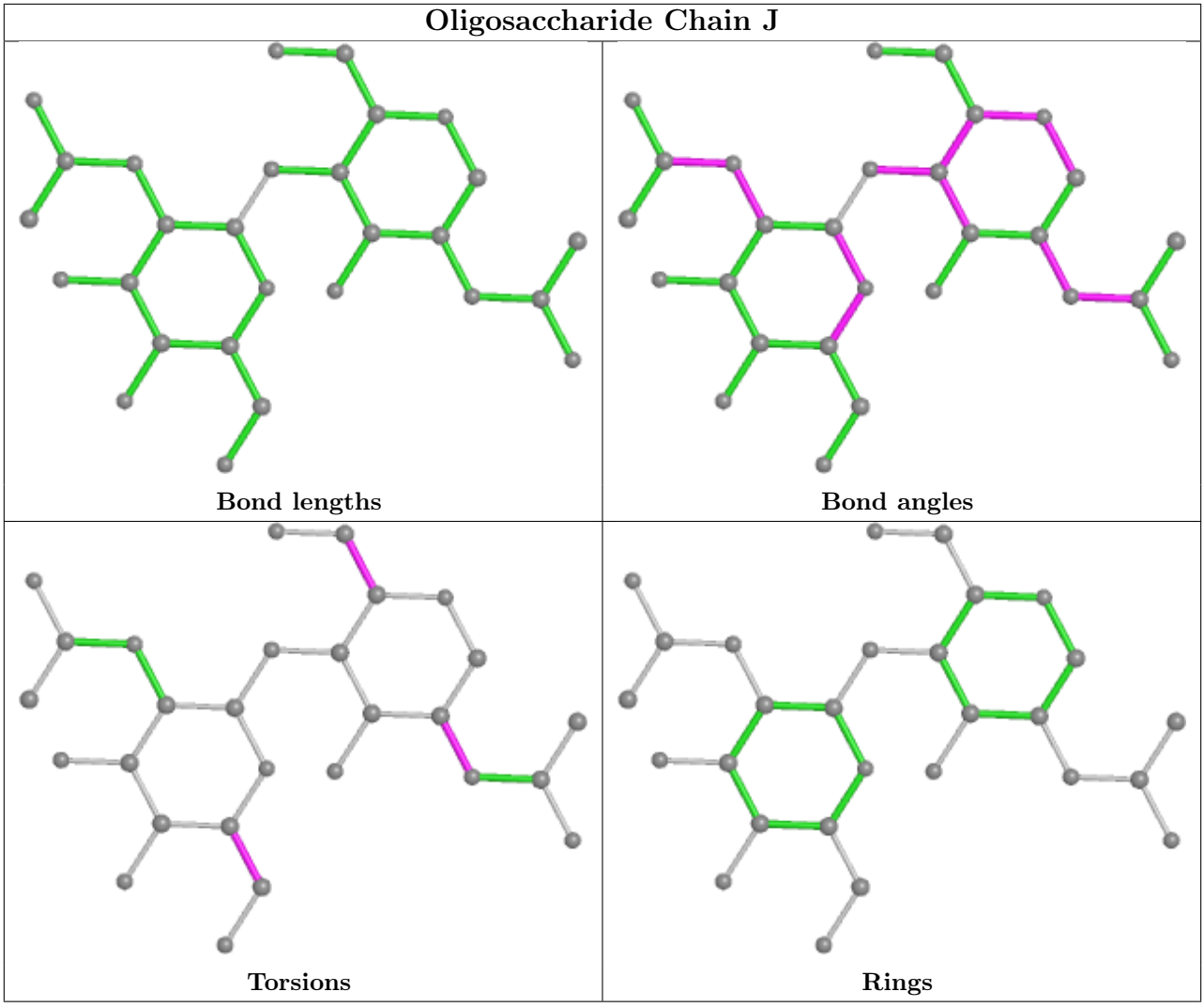
Bond angles



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

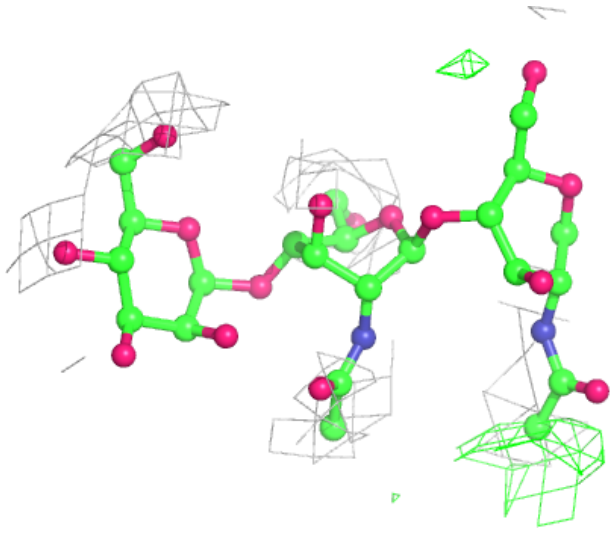
6.3 Carbohydrates

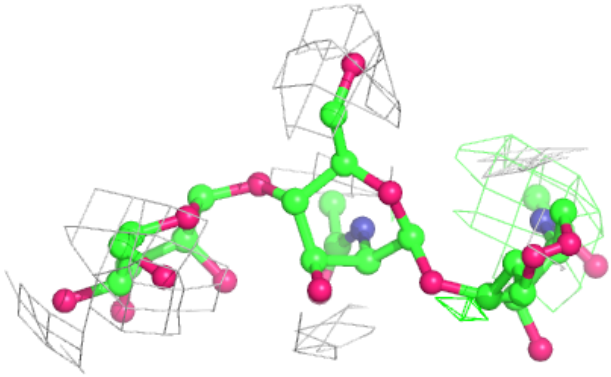
Unable to reproduce the depositors R factor - this section is therefore empty.

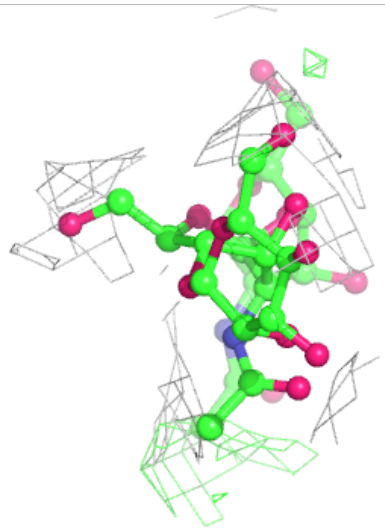
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain F:

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

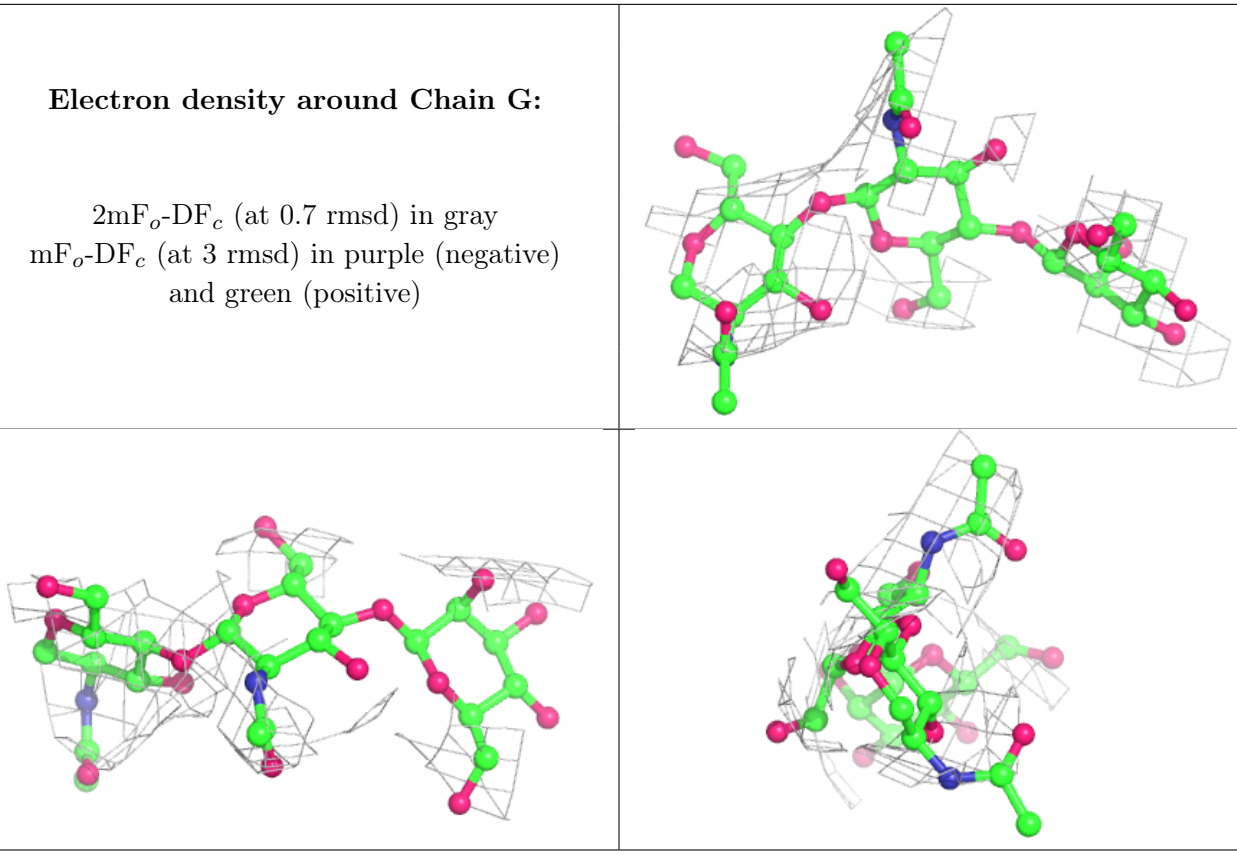






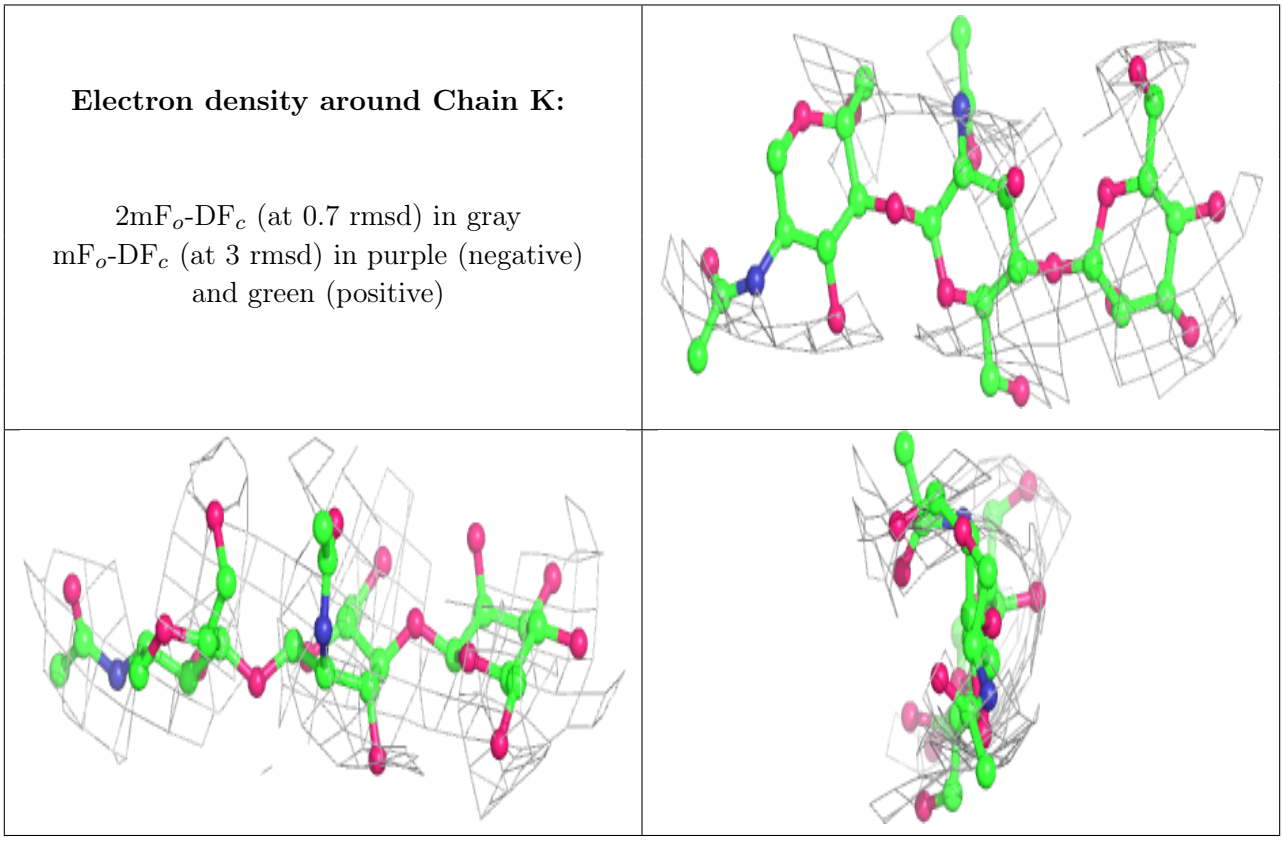
Electron density around Chain G:

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



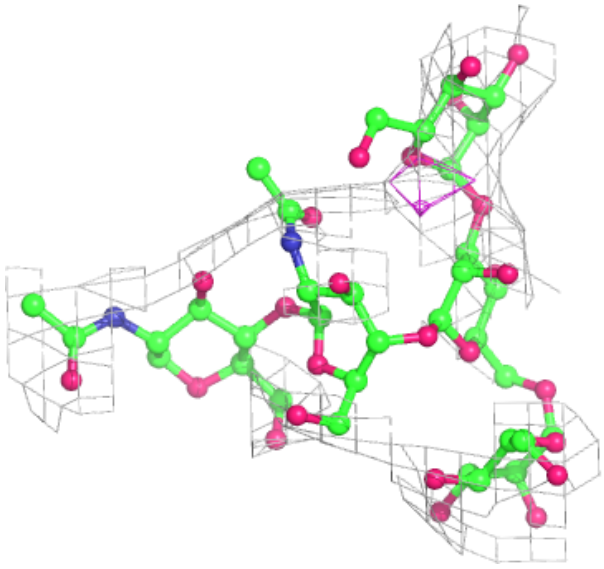
Electron density around Chain K:

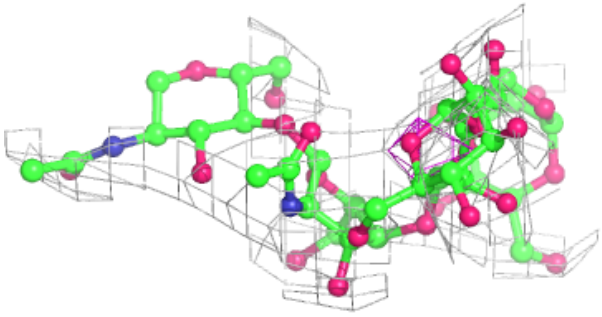
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

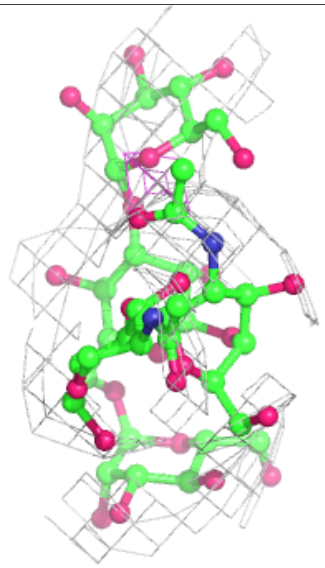


Electron density around Chain I:

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

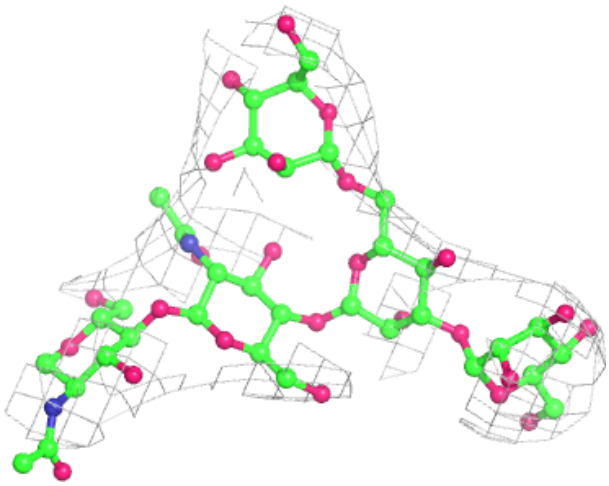


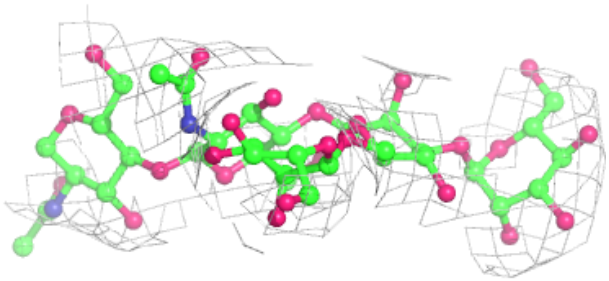


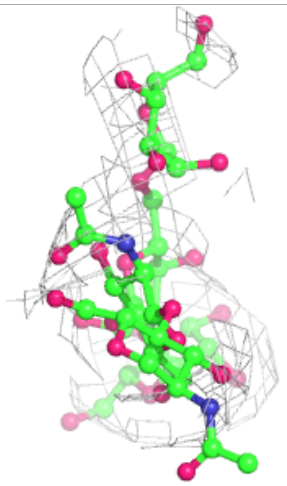


Electron density around Chain M:

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

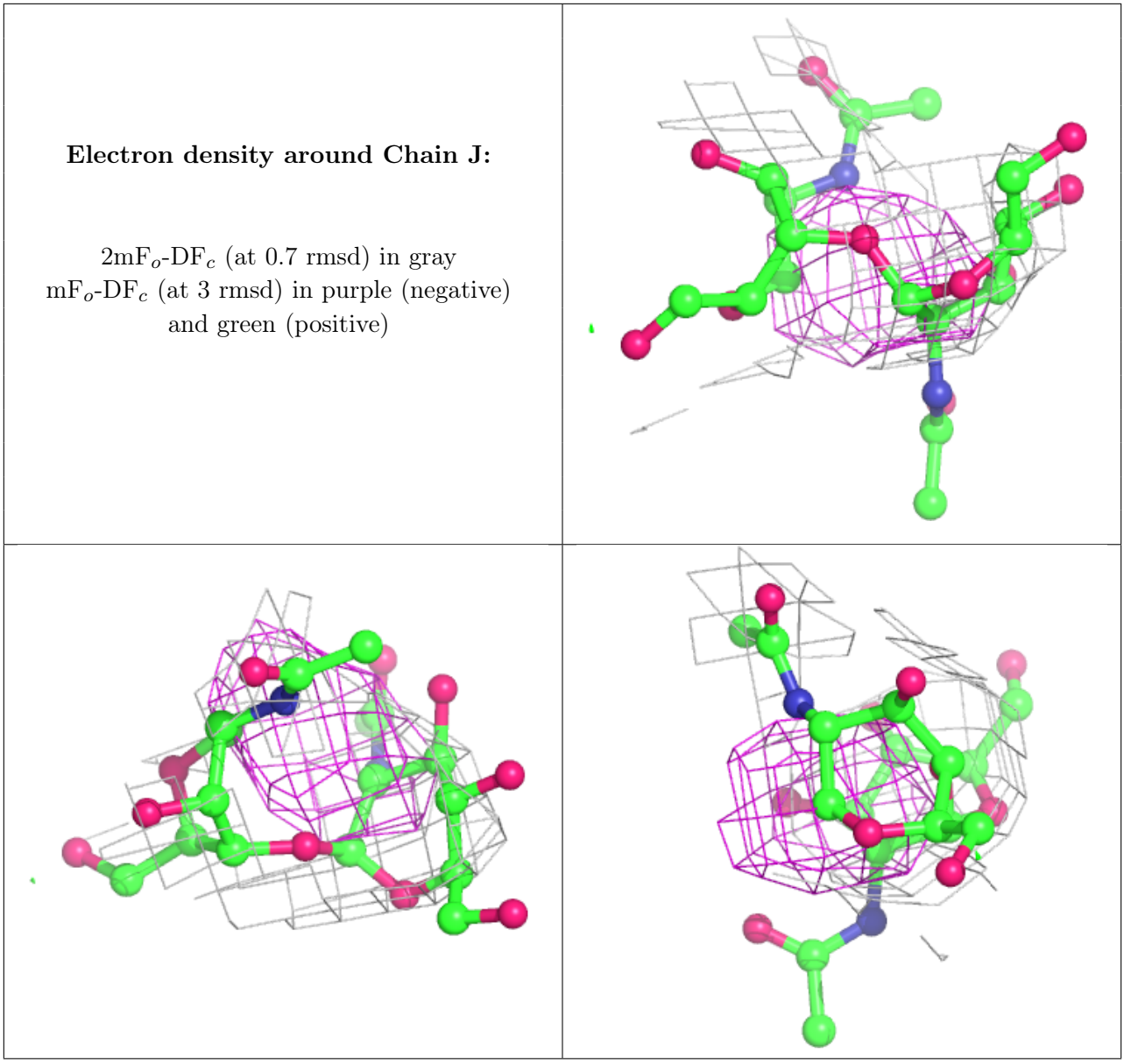






Electron density around Chain J:

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



6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.