Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 08:53 AM EDT

PDB ID	:	5W1O
Title	:	Crystal Structure of HPV16 L1 Pentamer Bound to Heparin Oligosaccharides
Authors	:	Dasgupta, J.; Chen, X.S.
Deposited on	:	2017-06-04
Resolution	:	2.80 Å(reported)

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

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

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

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

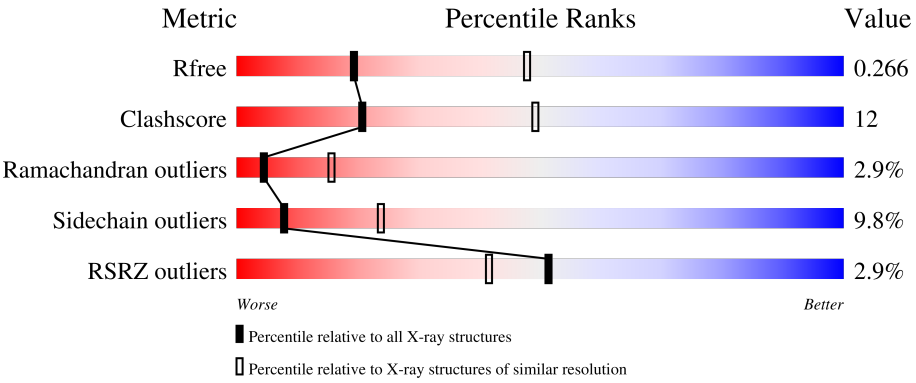
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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% 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	427	3% 69% 25% 5%
1	B	427	3% 71% 24%
1	C	427	2% 68% 26% 5%
1	D	427	4% 71% 25%
1	E	427	3% 70% 26%

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Mol	Chain	Length	Quality of chain
2	F	2	50% 50%
2	H	2	100%
2	I	2	100%
2	J	2	100%
2	K	2	50% 50%
2	L	2	50% 50%
2	M	2	50% 50%
2	N	2	50% 50%
2	O	2	100%
2	P	2	100%
3	G	6	33% 67%

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
2	JHM	F	1	-	-	X	X
2	IDS	F	2	-	-	-	X
2	JHM	H	1	-	-	X	X
2	IDS	H	2	-	-	-	X
2	JHM	I	1	-	-	X	X
2	IDS	I	2	-	-	X	X
2	JHM	J	1	-	-	X	X
2	IDS	J	2	-	-	X	X
2	JHM	K	1	-	-	-	X
2	IDS	K	2	-	-	-	X
2	JHM	L	1	-	-	-	X
2	IDS	L	2	-	-	-	X
2	JHM	M	1	-	-	X	X
2	IDS	M	2	-	-	-	X
2	JHM	N	1	-	-	-	X
2	IDS	N	2	-	-	-	X
2	JHM	O	1	-	-	-	X
2	IDS	O	2	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	JHM	P	1	-	-	X	X
2	IDS	P	2	-	-	-	X
3	JHM	G	1	-	-	-	X
3	IDS	G	2	-	-	-	X
3	JHM	G	3	-	-	-	X
3	IDS	G	4	-	-	-	X
3	JHM	G	5	-	-	-	X
3	IDS	G	6	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17224 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 Major capsid protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3344	2125	562	637	20			
1	B	427	Total	C	N	O	S	0	0	0
			3344	2125	562	637	20			
1	C	427	Total	C	N	O	S	0	0	0
			3344	2125	562	637	20			
1	D	425	Total	C	N	O	S	0	0	0
			3328	2114	560	634	20			
1	E	425	Total	C	N	O	S	0	0	0
			3327	2115	559	633	20			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	-	expression tag	UNP Q81007
A	432	GLY	-	linker	UNP Q81007
A	433	GLY	-	linker	UNP Q81007
A	434	GLY	-	linker	UNP Q81007
A	435	SER	-	linker	UNP Q81007
A	436	GLY	-	linker	UNP Q81007
A	437	ALA	-	linker	UNP Q81007
B	20	ALA	-	expression tag	UNP Q81007
B	432	GLY	-	linker	UNP Q81007
B	433	GLY	-	linker	UNP Q81007
B	434	GLY	-	linker	UNP Q81007
B	435	SER	-	linker	UNP Q81007
B	436	GLY	-	linker	UNP Q81007
B	437	ALA	-	linker	UNP Q81007
C	20	ALA	-	expression tag	UNP Q81007
C	432	GLY	-	linker	UNP Q81007
C	433	GLY	-	linker	UNP Q81007
C	434	GLY	-	linker	UNP Q81007
C	435	SER	-	linker	UNP Q81007

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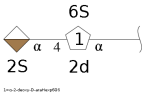
Chain	Residue	Modelled	Actual	Comment	Reference
C	436	GLY	-	linker	UNP Q81007
C	437	ALA	-	linker	UNP Q81007
D	20	ALA	-	expression tag	UNP Q81007
D	432	GLY	-	linker	UNP Q81007
D	433	GLY	-	linker	UNP Q81007
D	434	GLY	-	linker	UNP Q81007
D	435	SER	-	linker	UNP Q81007
D	436	GLY	-	linker	UNP Q81007
D	437	ALA	-	linker	UNP Q81007
E	20	ALA	-	expression tag	UNP Q81007
E	432	GLY	-	linker	UNP Q81007
E	433	GLY	-	linker	UNP Q81007
E	434	GLY	-	linker	UNP Q81007
E	435	SER	-	linker	UNP Q81007
E	436	GLY	-	linker	UNP Q81007
E	437	ALA	-	linker	UNP Q81007

- Molecule 2 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy -6-O-sulfo-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	H	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	I	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	J	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	K	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	L	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	M	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	N	2	Total	C	O	S	0	0	0
			30	12	16	2			

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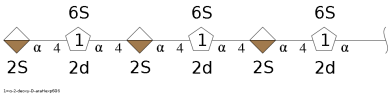
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	O	2	Total C O S 30 12 16 2	0	0	0
2	P	2	Total C O S 30 12 16 2	0	0	0

- Molecule 3 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	G	6	Total C O S 90 36 48 6	0	0	0

- Molecule 4 is water.

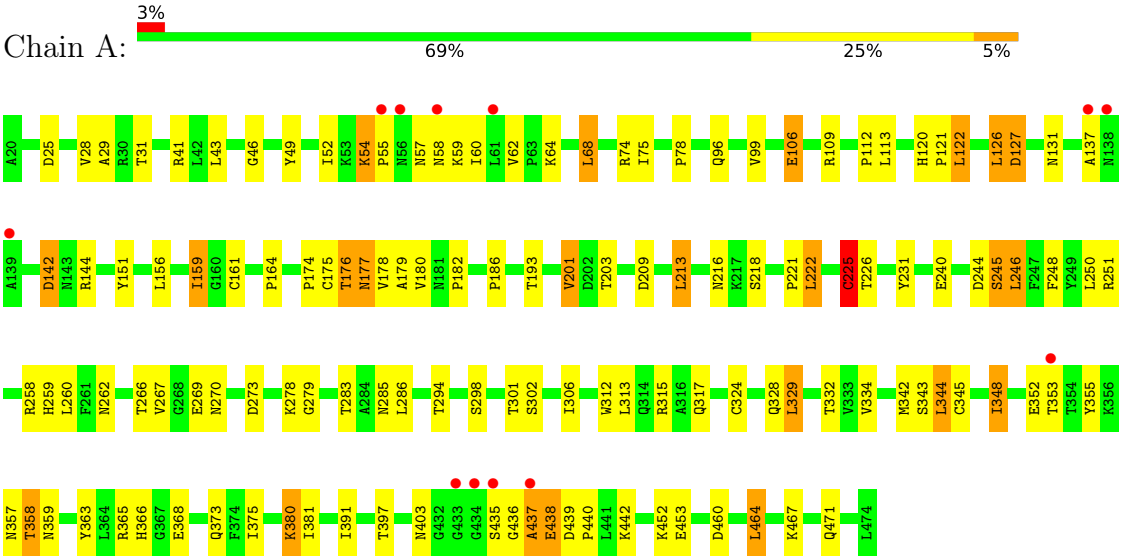
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	33	Total O 33 33	0	0
4	B	25	Total O 25 25	0	0
4	C	34	Total O 34 34	0	0
4	D	23	Total O 23 23	0	0
4	E	32	Total O 32 32	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

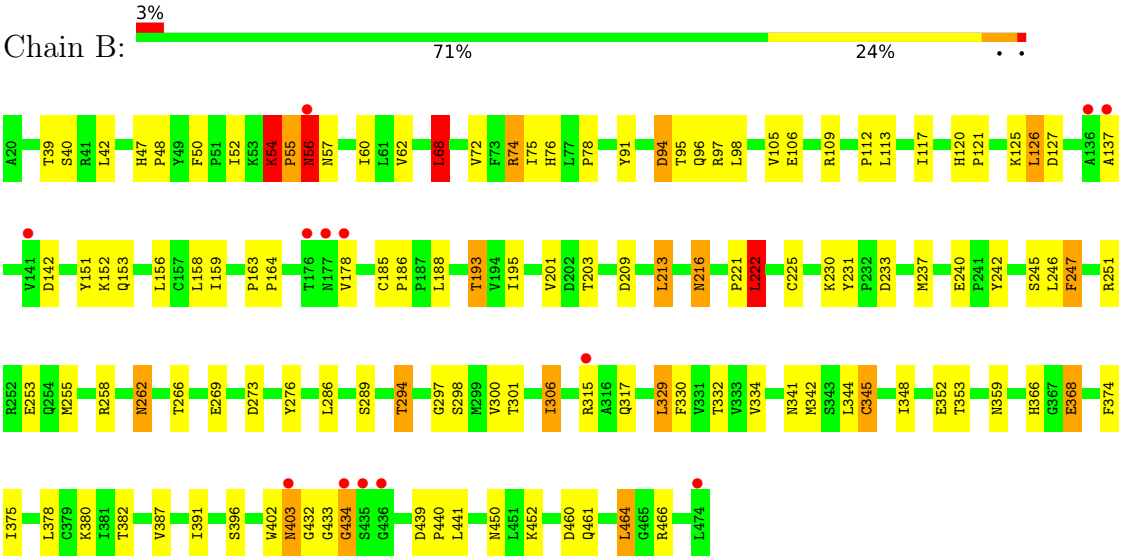
• Molecule 1: Major capsid protein L1

Chain A:



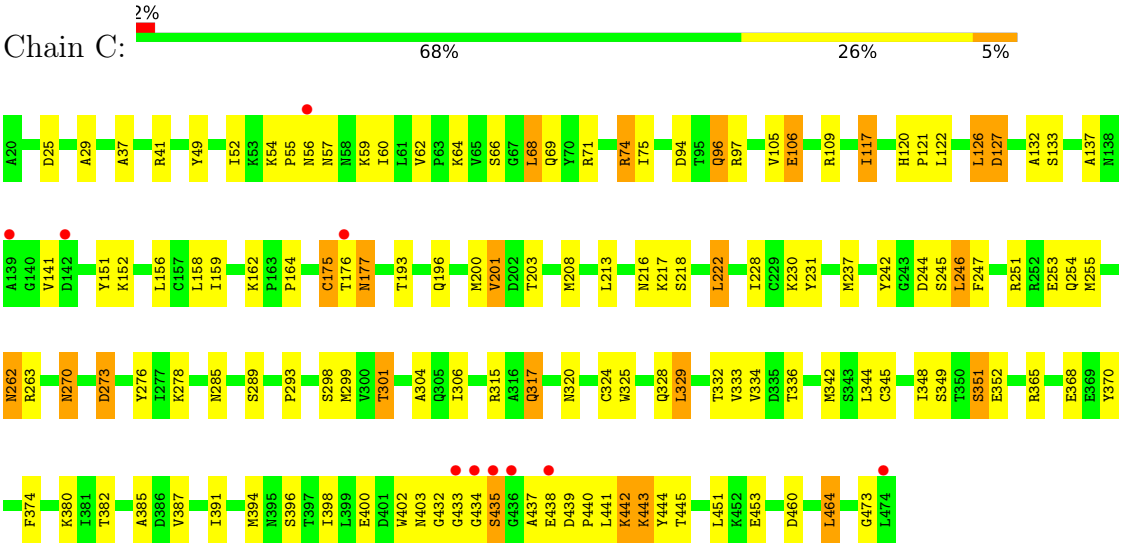
• Molecule 1: Major capsid protein L1

Chain B:



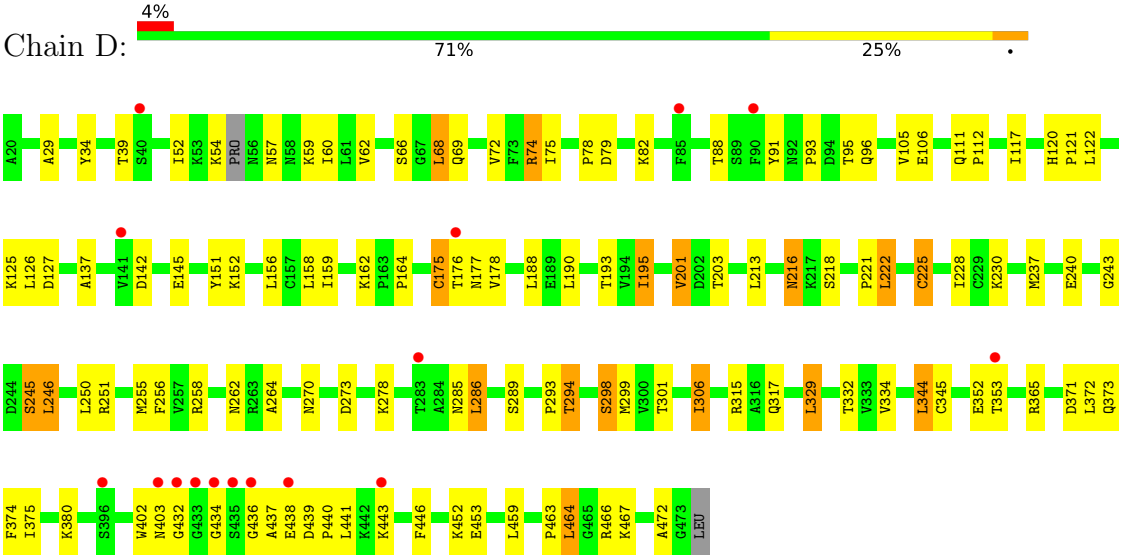
• Molecule 1: Major capsid protein L1

Chain C:



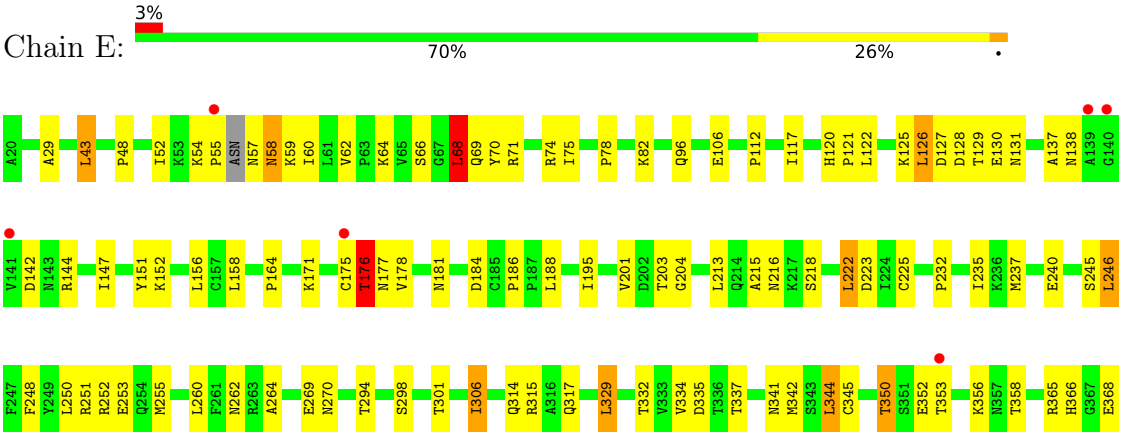
• Molecule 1: Major capsid protein L1

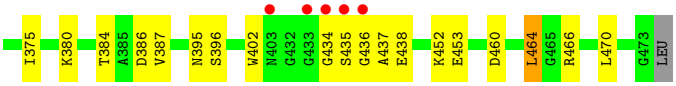
Chain D:



• Molecule 1: Major capsid protein L1

Chain E:



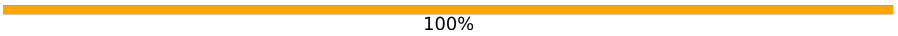


• Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain F:

• Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain H:



• Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain I:

• Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain J:

• Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain K:

• Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain L:

• Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain M:

• Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain N:

• Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain O:

• Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain P:

• Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.62Å 101.25Å 128.18Å 90.00° 90.63° 90.00°	Depositor
Resolution (Å)	47.43 – 2.80 47.43 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.43-2.80) 93.6 (47.43-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.224 , 0.270 0.222 , 0.266	Depositor DCC
R_{free} test set	3025 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 29.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -k,-h,-l 0.012 for k,h,-l 0.020 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	17224	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: JHM, IDS

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	0.46	1/3430 (0.0%)	0.62	1/4664 (0.0%)
1	B	0.48	1/3430 (0.0%)	0.63	2/4664 (0.0%)
1	C	0.45	0/3430	0.62	1/4664 (0.0%)
1	D	0.47	1/3412 (0.0%)	0.63	2/4638 (0.0%)
1	E	0.47	0/3412	0.64	1/4639 (0.0%)
All	All	0.47	3/17114 (0.0%)	0.63	7/23269 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	225	CYS	CB-SG	-6.74	1.70	1.82
1	A	225	CYS	CB-SG	-6.62	1.71	1.82
1	D	225	CYS	CB-SG	-5.21	1.73	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	68	LEU	CA-CB-CG	-6.95	99.31	115.30
1	E	68	LEU	CA-CB-CG	-6.34	100.73	115.30
1	A	246	LEU	CA-CB-CG	5.54	128.05	115.30
1	B	68	LEU	CA-CB-CG	-5.51	102.62	115.30
1	C	246	LEU	CA-CB-CG	5.46	127.86	115.30
1	D	246	LEU	CA-CB-CG	5.18	127.21	115.30
1	B	222	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3344	0	3240	90	6
1	B	3344	0	3240	89	1
1	C	3344	0	3240	103	7
1	D	3328	0	3220	71	0
1	E	3327	0	3222	74	0
2	F	30	0	14	22	0
2	H	30	0	14	13	0
2	I	30	0	14	16	0
2	J	30	0	13	12	10
2	K	30	0	13	5	0
2	L	30	0	14	5	0
2	M	30	0	14	6	0
2	N	30	0	14	4	1
2	O	30	0	14	8	0
2	P	30	0	14	12	0
3	G	90	0	39	11	1
4	A	33	0	0	5	0
4	B	25	0	0	4	0
4	C	34	0	0	10	0
4	D	23	0	0	2	0
4	E	32	0	0	6	0
All	All	17224	0	16339	412	13

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 (412) 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:B:266:THR:HG21	2:F:1:JHM:C6	1.21	1.63
1:B:266:THR:CG2	2:F:1:JHM:H6A	1.19	1.62
1:A:358:THR:CB	2:F:1:JHM:H1	1.30	1.56
1:A:358:THR:CG2	2:F:1:JHM:C1	1.82	1.55
1:E:452:LYS:NZ	2:P:1:JHM:C6	1.72	1.49
1:A:358:THR:CG2	2:F:1:JHM:H1	0.95	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:THR:CB	2:F:1:JHM:C1	1.96	1.36
1:E:452:LYS:NZ	2:P:1:JHM:H6A	1.05	1.35
2:O:1:JHM:O1	2:P:2:IDS:C4	1.73	1.35
1:A:358:THR:HB	2:F:1:JHM:C1	1.56	1.34
1:A:358:THR:HG22	2:F:1:JHM:C1	1.47	1.33
1:C:196:GLN:HE22	2:I:2:IDS:C6	1.12	1.30
2:L:2:IDS:C4	2:M:1:JHM:O1	1.81	1.28
1:A:358:THR:HB	2:F:1:JHM:O5	1.39	1.22
2:H:1:JHM:H1	2:I:2:IDS:O6B	1.35	1.20
1:C:196:GLN:NE2	2:I:2:IDS:C6	1.85	1.20
1:E:358:THR:HB	3:G:2:IDS:O6A	1.02	1.19
1:E:358:THR:CB	3:G:2:IDS:O6A	1.91	1.19
1:A:358:THR:HG22	2:F:1:JHM:O1	1.42	1.18
2:L:2:IDS:O2S	2:M:1:JHM:O8	1.62	1.18
1:C:55:PRO:HG3	2:J:1:JHM:C1	1.72	1.17
2:L:2:IDS:C4	2:M:1:JHM:C1	2.25	1.13
1:A:358:THR:HG21	2:F:1:JHM:H1	1.25	1.12
1:C:55:PRO:HG3	2:J:1:JHM:H1	1.32	1.09
1:E:452:LYS:HZ3	2:P:1:JHM:C6	1.46	1.08
1:C:55:PRO:HG3	2:J:1:JHM:O5	1.55	1.07
2:H:1:JHM:H1	2:I:2:IDS:C6	1.85	1.04
1:A:358:THR:HG22	2:F:1:JHM:HO1	1.24	1.03
2:N:1:JHM:O1	2:O:2:IDS:C4	2.07	1.02
1:C:196:GLN:NE2	2:I:2:IDS:O6B	1.92	1.01
1:E:452:LYS:HZ2	2:P:1:JHM:H6	1.26	1.01
1:E:452:LYS:HZ2	2:P:1:JHM:C6	1.67	0.98
1:D:285:ASN:ND2	2:K:1:JHM:O9	1.97	0.97
1:E:358:THR:HB	3:G:2:IDS:C6	1.92	0.97
1:E:452:LYS:NZ	2:P:1:JHM:H6	1.77	0.94
1:C:443:LYS:NZ	2:I:1:JHM:O8	2.01	0.94
1:E:71:ARG:NH2	4:E:601:HOH:O	2.02	0.93
2:H:1:JHM:C1	2:I:2:IDS:O6B	2.17	0.93
1:D:285:ASN:HA	2:K:1:JHM:O9	1.69	0.91
1:A:358:THR:CB	2:F:1:JHM:O5	2.06	0.88
1:C:55:PRO:CG	2:J:1:JHM:O5	2.22	0.87
2:N:1:JHM:H6A	2:O:2:IDS:O2S	1.76	0.85
1:E:452:LYS:HZ1	2:P:1:JHM:H6A	1.40	0.85
1:E:452:LYS:HZ1	2:P:1:JHM:C6	1.84	0.85
2:O:1:JHM:C1	2:P:2:IDS:C4	2.53	0.85
2:O:1:JHM:HO1	2:P:2:IDS:C4	1.90	0.84
1:E:270:ASN:ND2	2:M:1:JHM:O9	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:THR:HG21	2:H:1:JHM:O7	1.79	0.81
1:C:444:TYR:HE2	2:I:1:JHM:H2A	1.46	0.81
1:C:334:VAL:O	4:C:601:HOH:O	1.98	0.81
1:C:263:ARG:N	4:C:602:HOH:O	2.08	0.80
1:B:266:THR:CG2	2:F:1:JHM:C6	2.06	0.80
1:C:444:TYR:CE2	2:I:1:JHM:H2	2.18	0.78
1:E:54:LYS:HD3	1:E:55:PRO:HD2	1.65	0.78
1:C:444:TYR:CE2	2:I:1:JHM:C2	2.67	0.78
1:D:375:ILE:HG12	1:D:464:LEU:HD13	1.67	0.77
1:C:156:LEU:O	4:C:601:HOH:O	2.02	0.76
1:D:285:ASN:HA	2:K:1:JHM:S	2.27	0.74
1:E:358:THR:HG1	3:G:1:JHM:HO3	1.06	0.74
1:A:358:THR:CA	2:F:1:JHM:O5	2.36	0.74
1:C:54:LYS:HG3	1:C:55:PRO:HD2	1.70	0.74
1:C:126:LEU:HB3	1:C:262:ASN:HB3	1.70	0.74
1:D:345:CYS:SG	4:E:602:HOH:O	2.45	0.74
2:N:1:JHM:C6	2:O:2:IDS:O2S	2.36	0.73
1:C:55:PRO:CG	2:J:1:JHM:H1	2.15	0.73
1:C:55:PRO:CG	2:J:1:JHM:C1	2.62	0.72
1:D:68:LEU:HD13	1:D:151:TYR:HD1	1.54	0.72
1:A:358:THR:HA	2:F:1:JHM:O5	1.89	0.72
1:C:29:ALA:HB3	1:C:380:LYS:HG3	1.71	0.71
1:B:126:LEU:HB3	1:B:262:ASN:HB3	1.72	0.71
1:E:375:ILE:HG12	1:E:464:LEU:HD13	1.70	0.71
1:E:69:GLN:OE1	4:E:601:HOH:O	2.09	0.70
1:B:56:ASN:N	1:B:56:ASN:OD1	2.24	0.70
1:E:215:ALA:N	4:E:602:HOH:O	2.16	0.70
1:B:240:GLU:OE2	1:B:245:SER:OG	2.09	0.70
1:B:402:TRP:O	1:B:432:GLY:N	2.25	0.69
1:E:358:THR:OG1	3:G:1:JHM:O3	1.91	0.69
1:C:444:TYR:HE2	2:I:1:JHM:C2	2.03	0.69
1:B:266:THR:HG21	2:F:1:JHM:C5	2.19	0.69
1:D:240:GLU:OE2	1:D:245:SER:OG	2.08	0.69
1:B:345:CYS:SG	1:C:216:ASN:HB2	2.34	0.68
2:L:2:IDS:C4	2:M:1:JHM:O5	2.41	0.68
1:A:345:CYS:SG	1:B:216:ASN:HB2	2.34	0.68
1:A:25:ASP:OD1	4:A:601:HOH:O	2.10	0.68
1:C:270:ASN:O	4:C:603:HOH:O	2.12	0.67
1:D:175:CYS:O	1:D:177:ASN:N	2.27	0.67
1:B:440:PRO:O	4:B:601:HOH:O	2.13	0.66
1:A:375:ILE:HG12	1:A:464:LEU:HD13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:GLY:O	1:A:438:GLU:N	2.28	0.66
1:C:59:LYS:O	4:C:604:HOH:O	2.13	0.65
1:D:54:LYS:HB3	1:D:57:ASN:HB2	1.79	0.65
1:D:298:SER:N	4:D:602:HOH:O	2.29	0.65
1:C:55:PRO:HB3	2:J:1:JHM:C6	2.28	0.64
1:C:345:CYS:SG	1:D:216:ASN:HB2	2.38	0.64
1:A:373:GLN:OE1	4:A:602:HOH:O	2.15	0.63
1:B:375:ILE:HG12	1:B:464:LEU:HD13	1.80	0.63
1:E:175:CYS:O	1:E:177:ASN:N	2.30	0.62
1:B:55:PRO:HB2	1:B:56:ASN:OD1	1.99	0.62
1:B:460:ASP:HB3	1:B:461:GLN:HE21	1.63	0.62
1:E:204:GLY:HA2	1:E:255:MET:HE2	1.81	0.62
1:B:52:ILE:HB	1:B:62:VAL:HB	1.81	0.62
1:C:55:PRO:HB3	2:J:1:JHM:O6	2.00	0.62
1:D:402:TRP:O	1:D:432:GLY:N	2.32	0.62
1:B:266:THR:CG2	2:F:1:JHM:C5	2.77	0.61
1:E:29:ALA:HB3	1:E:380:LYS:HG3	1.82	0.61
1:A:106:GLU:OE2	1:A:467:LYS:NZ	2.33	0.61
2:L:2:IDS:C4	2:M:1:JHM:H1	2.29	0.61
1:C:75:ILE:HB	1:C:329:LEU:HB3	1.82	0.61
1:D:74:ARG:NH2	1:D:439:ASP:OD2	2.33	0.60
1:D:286:LEU:N	2:K:1:JHM:O8	2.36	0.59
1:E:240:GLU:OE2	1:E:245:SER:OG	2.14	0.59
1:A:240:GLU:OE2	1:A:245:SER:OG	2.17	0.59
1:C:55:PRO:HB3	2:J:1:JHM:O5	2.02	0.59
1:A:177:ASN:OD1	1:A:177:ASN:N	2.36	0.59
1:B:96:GLN:HB3	1:B:382:THR:HA	1.84	0.58
1:B:113:LEU:HD22	1:C:253:GLU:HG3	1.85	0.58
1:A:113:LEU:HD22	1:B:253:GLU:HG3	1.84	0.58
1:C:121:PRO:HG3	1:D:289:SER:HB3	1.85	0.58
1:D:344:LEU:HD12	1:E:186:PRO:HG2	1.85	0.58
1:A:269:GLU:OE1	1:E:365:ARG:NH2	2.36	0.58
1:C:55:PRO:CB	2:J:1:JHM:O5	2.50	0.58
1:B:341:ASN:HD22	1:B:366:HIS:HB2	1.68	0.58
1:B:258:ARG:HB3	1:B:294:THR:HG22	1.86	0.58
1:A:126:LEU:HB3	1:A:262:ASN:HB3	1.86	0.57
1:C:52:ILE:HB	1:C:62:VAL:HB	1.85	0.57
1:C:57:ASN:ND2	1:C:59:LYS:HB3	2.19	0.57
1:C:432:GLY:O	1:C:434:GLY:N	2.37	0.57
1:C:151:TYR:CG	1:C:203:THR:HB	2.39	0.57
1:C:200:MET:SD	2:H:2:IDS:O6A	2.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ILE:HG22	1:B:359:ASN:OD1	2.04	0.57
1:A:343:SER:O	4:A:603:HOH:O	2.16	0.57
1:C:97:ARG:HH21	1:C:403:ASN:HB2	1.69	0.57
1:E:466:ARG:NH2	4:E:606:HOH:O	2.38	0.57
1:A:260:LEU:HD23	1:E:117:ILE:HG13	1.86	0.57
1:C:444:TYR:CE2	2:I:1:JHM:H2A	2.30	0.57
1:B:266:THR:CB	2:F:1:JHM:H6A	2.20	0.56
1:C:109:ARG:HH12	1:C:368:GLU:HG3	1.70	0.56
1:E:126:LEU:HD13	1:E:264:ALA:HB2	1.85	0.56
1:A:344:LEU:HD12	1:B:186:PRO:HG2	1.86	0.56
1:D:158:LEU:HB2	1:D:332:THR:HB	1.86	0.56
1:C:117:ILE:HG21	1:D:293:PRO:HD3	1.86	0.56
1:E:78:PRO:HD3	1:E:452:LYS:HA	1.88	0.56
1:C:244:ASP:OD1	1:C:320:ASN:ND2	2.39	0.56
1:C:175:CYS:HB3	1:C:177:ASN:HB2	1.86	0.56
1:A:175:CYS:O	1:A:177:ASN:N	2.38	0.55
1:C:285:ASN:HA	4:C:613:HOH:O	2.05	0.55
1:A:112:PRO:HB3	1:B:231:TYR:CD1	2.41	0.55
1:D:68:LEU:O	1:D:201:VAL:HG23	2.06	0.55
2:H:1:JHM:C2	2:I:2:IDS:O6B	2.55	0.55
1:E:75:ILE:HB	1:E:329:LEU:HB3	1.87	0.55
1:D:68:LEU:HD13	1:D:151:TYR:CD1	2.39	0.55
1:B:74:ARG:NH2	1:B:439:ASP:OD2	2.39	0.55
1:C:175:CYS:O	1:C:177:ASN:N	2.40	0.55
1:C:273:ASP:OD2	1:C:273:ASP:N	2.40	0.55
1:E:57:ASN:O	1:E:59:LYS:N	2.40	0.55
1:C:217:LYS:NZ	4:C:608:HOH:O	2.38	0.54
1:A:29:ALA:HB3	1:A:380:LYS:HG3	1.89	0.54
1:E:358:THR:CB	3:G:1:JHM:HO3	2.17	0.54
1:D:52:ILE:HB	1:D:62:VAL:HB	1.90	0.54
1:D:345:CYS:O	4:E:602:HOH:O	2.18	0.54
1:C:68:LEU:O	1:C:201:VAL:HG23	2.07	0.54
1:E:64:LYS:NZ	1:E:223:ASP:O	2.40	0.54
1:C:273:ASP:HA	1:C:276:TYR:CE2	2.43	0.54
1:A:78:PRO:HD3	1:A:452:LYS:HA	1.90	0.54
1:B:273:ASP:HA	1:B:276:TYR:CE2	2.43	0.54
1:E:358:THR:CB	3:G:1:JHM:O3	2.56	0.54
1:E:358:THR:CA	3:G:2:IDS:O6A	2.54	0.53
1:B:120:HIS:CD2	1:B:222:LEU:HD13	2.43	0.53
1:D:151:TYR:CD2	1:D:203:THR:HB	2.44	0.53
1:C:349:SER:OG	1:C:351:SER:OG	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:SER:HB3	1:D:69:GLN:HG3	1.91	0.53
1:D:285:ASN:CA	2:K:1:JHM:O9	2.51	0.53
1:B:75:ILE:HB	1:B:329:LEU:HB3	1.90	0.53
1:A:358:THR:HG21	2:F:1:JHM:C1	2.04	0.53
1:B:266:THR:HG22	2:F:1:JHM:C6	2.26	0.52
1:D:345:CYS:SG	1:E:216:ASN:HB2	2.49	0.52
1:B:193:THR:HG21	1:B:230:LYS:HD2	1.91	0.52
2:O:1:JHM:H1	2:P:2:IDS:C4	2.36	0.52
1:E:158:LEU:HB2	1:E:332:THR:HB	1.92	0.52
1:C:54:LYS:HB3	1:C:57:ASN:HB3	1.91	0.52
1:D:122:LEU:O	1:D:218:SER:HB3	2.10	0.52
1:B:39:THR:HB	1:B:42:LEU:HD21	1.91	0.52
1:C:25:ASP:OD1	4:C:606:HOH:O	2.18	0.52
1:B:72:VAL:HG22	1:B:332:THR:HG23	1.90	0.51
1:B:209:ASP:O	1:B:213:LEU:HB2	2.10	0.51
1:B:164:PRO:HG2	1:B:195:ILE:HB	1.92	0.51
1:A:52:ILE:HA	4:A:607:HOH:O	2.10	0.51
1:A:186:PRO:HG2	1:E:344:LEU:HD12	1.93	0.51
1:A:231:TYR:CD1	1:E:112:PRO:HB3	2.46	0.51
1:A:266:THR:HB	3:G:3:JHM:O7	2.11	0.51
1:A:365:ARG:NH2	1:B:269:GLU:OE1	2.43	0.51
1:E:252:ARG:HD2	1:E:306:ILE:HD11	1.91	0.51
1:E:164:PRO:HG2	1:E:195:ILE:HB	1.93	0.51
1:A:52:ILE:HB	1:A:62:VAL:HB	1.93	0.51
1:A:75:ILE:HB	1:A:329:LEU:HB3	1.92	0.51
1:C:158:LEU:HB2	1:C:332:THR:HB	1.93	0.51
2:H:1:JHM:H1	2:I:2:IDS:C4	2.41	0.51
1:C:216:ASN:OD1	1:C:218:SER:HB2	2.11	0.50
1:C:69:GLN:OE1	1:C:71:ARG:NH2	2.45	0.50
1:D:436:GLY:O	1:D:438:GLU:N	2.43	0.50
1:B:152:LYS:HB2	1:B:255:MET:HG3	1.94	0.50
1:D:466:ARG:NH2	4:D:606:HOH:O	2.45	0.50
1:B:387:VAL:HG13	1:B:391:ILE:HD13	1.94	0.50
1:D:162:LYS:HB2	1:D:245:SER:HA	1.93	0.50
1:A:358:THR:CA	2:F:1:JHM:C1	2.83	0.50
1:C:325:TRP:HB3	1:C:398:ILE:CD1	2.42	0.50
1:D:240:GLU:HG2	1:D:243:GLY:H	1.76	0.50
1:A:363:TYR:CE2	1:B:185:CYS:HB2	2.46	0.50
1:B:233:ASP:OD1	4:B:602:HOH:O	2.20	0.50
1:B:159:ILE:HG22	1:B:247:PHE:HE1	1.77	0.49
1:C:64:LYS:HE3	2:H:2:IDS:C4	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:VAL:O	1:C:391:ILE:HG12	2.12	0.49
1:D:298:SER:OG	1:D:299:MET:N	2.44	0.49
1:B:97:ARG:HH21	1:B:403:ASN:HB2	1.76	0.49
1:D:120:HIS:HB2	1:D:221:PRO:HA	1.94	0.49
1:A:121:PRO:HD3	1:A:222:LEU:HD21	1.93	0.49
1:A:176:THR:O	1:A:176:THR:OG1	2.22	0.49
1:D:72:VAL:HG22	1:D:332:THR:HG23	1.94	0.49
1:D:228:ILE:HG22	1:D:230:LYS:HG2	1.94	0.49
1:A:122:LEU:O	1:A:218:SER:HB3	2.11	0.49
1:C:385:ALA:N	4:C:612:HOH:O	2.45	0.49
1:D:164:PRO:HG2	1:D:195:ILE:HB	1.95	0.49
1:E:201:VAL:HG21	1:E:334:VAL:HG11	1.93	0.49
1:B:237:MET:SD	1:B:246:LEU:HD23	2.53	0.49
1:B:246:LEU:HD12	1:B:246:LEU:O	2.13	0.49
1:C:64:LYS:HD2	2:H:2:IDS:C4	2.43	0.48
1:D:126:LEU:HB3	1:D:262:ASN:HB3	1.95	0.48
1:D:270:ASN:OD1	2:J:2:IDS:C3	2.58	0.48
1:E:171:LYS:HG3	1:E:186:PRO:HB2	1.94	0.48
2:H:1:JHM:O1	2:I:2:IDS:C4	2.61	0.48
1:B:121:PRO:HG3	1:C:289:SER:HB3	1.96	0.48
1:B:353:THR:N	4:B:603:HOH:O	2.28	0.48
1:B:153:GLN:OE1	1:B:300:VAL:HG12	2.14	0.48
1:E:151:TYR:CD2	1:E:203:THR:HB	2.48	0.48
1:E:434:GLY:O	1:E:436:GLY:N	2.46	0.48
1:B:117:ILE:HG21	1:C:293:PRO:HD3	1.94	0.48
1:E:130:GLU:HB2	1:E:260:LEU:HB2	1.95	0.48
1:A:68:LEU:O	1:A:201:VAL:HG23	2.14	0.48
1:A:109:ARG:HH12	1:A:368:GLU:HG3	1.79	0.48
1:B:68:LEU:HD13	1:B:151:TYR:HD1	1.79	0.48
1:B:94:ASP:OD1	1:B:94:ASP:N	2.47	0.48
1:B:121:PRO:HD3	1:B:222:LEU:HD21	1.96	0.48
1:B:164:PRO:HG3	1:B:332:THR:OG1	2.14	0.48
1:B:341:ASN:ND2	1:B:366:HIS:HB2	2.29	0.48
1:D:68:LEU:CD1	1:D:151:TYR:HD1	2.24	0.48
1:D:79:ASP:HB3	1:D:82:LYS:HB2	1.96	0.48
1:B:152:LYS:HE3	1:B:253:GLU:HB2	1.96	0.47
1:A:142:ASP:OD1	1:A:144:ARG:NH2	2.43	0.47
1:B:68:LEU:O	1:B:201:VAL:HG23	2.14	0.47
1:A:28:VAL:HG13	1:A:381:ILE:HD11	1.97	0.47
1:B:109:ARG:HH12	1:B:368:GLU:HG3	1.80	0.47
1:C:162:LYS:HB2	1:C:245:SER:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:LEU:O	1:C:246:LEU:HD12	2.14	0.47
1:E:366:HIS:HE1	1:E:368:GLU:OE1	1.98	0.47
1:A:267:VAL:HG11	1:A:270:ASN:HA	1.97	0.47
1:C:156:LEU:N	4:C:601:HOH:O	2.21	0.47
1:D:371:ASP:OD2	1:D:373:GLN:NE2	2.47	0.47
2:N:1:JHM:H6	2:O:2:IDS:O2S	2.14	0.47
1:E:436:GLY:O	1:E:438:GLU:N	2.48	0.47
1:C:442:LYS:HB3	1:C:442:LYS:HE3	1.72	0.47
1:D:156:LEU:HA	1:D:250:LEU:O	2.15	0.47
1:A:57:ASN:OD1	1:A:59:LYS:HB3	2.15	0.46
1:A:120:HIS:ND1	1:A:121:PRO:HD2	2.29	0.46
1:A:225:CYS:SG	1:A:226:THR:HG23	2.55	0.46
1:A:258:ARG:HG3	1:A:259:HIS:CD2	2.50	0.46
1:D:443:LYS:HE2	1:D:443:LYS:HA	1.96	0.46
1:C:156:LEU:HG	1:C:334:VAL:HB	1.97	0.46
1:D:121:PRO:HD3	1:D:222:LEU:HD21	1.97	0.46
1:C:57:ASN:HD21	1:C:59:LYS:HB3	1.79	0.46
1:E:181:ASN:HB2	1:E:184:ASP:OD1	2.15	0.46
1:B:125:LYS:O	1:B:125:LYS:HD3	2.16	0.46
1:E:384:THR:OG1	1:E:387:VAL:HG23	2.16	0.46
1:A:126:LEU:HG	1:A:127:ASP:OD2	2.16	0.46
1:B:105:VAL:HG22	1:B:374:PHE:CD2	2.50	0.46
1:A:267:VAL:O	3:G:3:JHM:O8	2.33	0.46
1:A:246:LEU:O	1:A:246:LEU:HD12	2.16	0.46
1:C:365:ARG:HG3	1:D:188:LEU:HD21	1.97	0.46
1:C:96:GLN:HB3	1:C:382:THR:HA	1.98	0.45
1:D:29:ALA:HB3	1:D:380:LYS:HG3	1.97	0.45
1:E:122:LEU:HD13	1:E:144:ARG:NH2	2.30	0.45
1:A:54:LYS:HB3	1:A:57:ASN:HB3	1.97	0.45
1:A:260:LEU:HB3	1:E:117:ILE:HD11	1.99	0.45
1:A:278:LYS:HB2	1:D:353:THR:O	2.16	0.45
1:C:105:VAL:HG22	1:C:374:PHE:CD2	2.51	0.45
1:A:46:GLY:O	1:A:365:ARG:HD3	2.17	0.45
1:A:201:VAL:HG21	1:A:334:VAL:HG11	1.99	0.45
1:C:333:VAL:HG11	1:C:370:TYR:HE2	1.80	0.45
1:E:125:LYS:HD2	1:E:147:ILE:HD11	1.98	0.45
1:A:49:TYR:O	1:A:64:LYS:HE2	2.17	0.45
1:A:164:PRO:HG3	1:A:332:THR:OG1	2.16	0.45
1:B:300:VAL:O	1:C:254:GLN:HA	2.16	0.45
1:A:156:LEU:HA	1:A:250:LEU:O	2.17	0.45
1:B:68:LEU:HD22	1:B:203:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:VAL:HG21	1:D:334:VAL:HG11	1.98	0.45
1:E:120:HIS:CD2	1:E:222:LEU:HD13	2.52	0.45
1:B:156:LEU:HG	1:B:334:VAL:HB	1.98	0.45
1:C:228:ILE:HG22	1:C:230:LYS:HG2	1.98	0.45
1:C:242:TYR:CD2	1:C:394:MET:HG3	2.52	0.45
1:D:152:LYS:HB2	1:D:255:MET:HG3	1.99	0.45
1:A:266:THR:HG23	1:E:358:THR:HA	1.98	0.45
1:B:98:LEU:HD13	1:B:378:LEU:HD11	1.99	0.45
1:E:48:PRO:HB3	1:E:341:ASN:ND2	2.32	0.45
1:E:156:LEU:HA	1:E:250:LEU:O	2.17	0.45
1:C:120:HIS:ND1	1:C:121:PRO:HD2	2.31	0.45
1:E:122:LEU:O	1:E:218:SER:HB3	2.16	0.45
1:B:97:ARG:HD2	1:B:402:TRP:HB3	1.99	0.44
1:B:306:ILE:HD13	1:B:306:ILE:HA	1.70	0.44
2:H:1:JHM:C1	2:I:2:IDS:C4	2.95	0.44
1:A:58:ASN:OD1	1:A:58:ASN:N	2.50	0.44
1:C:106:GLU:HB2	1:C:464:LEU:HG	2.00	0.44
1:C:396:SER:O	1:C:400:GLU:HG3	2.18	0.44
1:A:312:TRP:NE1	1:A:471:GLN:HG3	2.31	0.44
1:C:152:LYS:HB2	1:C:255:MET:HG3	1.99	0.44
1:C:464:LEU:HD23	1:C:464:LEU:HA	1.87	0.44
1:B:466:ARG:HD2	1:C:317:GLN:O	2.18	0.44
1:C:121:PRO:HD3	1:C:222:LEU:HD21	1.99	0.44
1:C:164:PRO:HG3	1:C:332:THR:OG1	2.17	0.44
1:E:129:THR:HG21	1:E:262:ASN:OD1	2.17	0.44
1:D:365:ARG:NH2	1:E:269:GLU:OE2	2.50	0.44
1:C:237:MET:SD	1:C:246:LEU:HD23	2.58	0.44
1:C:49:TYR:O	1:C:64:LYS:HE2	2.18	0.44
1:C:97:ARG:NH2	1:C:403:ASN:HB2	2.31	0.44
1:D:39:THR:HG23	1:D:372:LEU:HB2	2.00	0.44
1:E:151:TYR:CG	1:E:203:THR:HB	2.53	0.44
1:B:151:TYR:CD2	1:B:203:THR:HB	2.53	0.44
1:C:242:TYR:CE2	1:C:394:MET:HG3	2.53	0.44
1:D:125:LYS:HD3	1:D:145:GLU:HG3	1.99	0.44
1:A:175:CYS:C	1:A:177:ASN:H	2.21	0.44
1:A:209:ASP:O	1:A:213:LEU:HB2	2.18	0.44
1:B:125:LYS:NZ	1:C:132:ALA:O	2.50	0.44
1:C:440:PRO:HG2	1:C:441:LEU:HD12	1.99	0.44
1:C:445:THR:CG2	2:H:1:JHM:O7	2.59	0.44
1:B:163:PRO:HD3	1:B:330:PHE:CE1	2.53	0.43
1:D:75:ILE:HB	1:D:329:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ASN:OD1	2:J:2:IDS:H3	2.17	0.43
1:E:152:LYS:HE3	1:E:253:GLU:HB2	2.00	0.43
1:A:28:VAL:HG13	1:A:381:ILE:CD1	2.48	0.43
1:E:52:ILE:HB	1:E:62:VAL:HB	1.99	0.43
1:D:105:VAL:HG22	1:D:374:PHE:CD2	2.54	0.43
1:A:285:ASN:HB2	4:A:609:HOH:O	2.18	0.43
1:E:176:THR:HG23	1:E:176:THR:O	2.19	0.43
1:D:463:PRO:O	1:D:467:LYS:HG3	2.18	0.43
1:C:301:THR:HG23	1:C:304:ALA:HB3	2.01	0.43
1:D:258:ARG:HB3	1:D:294:THR:HG22	2.00	0.43
1:B:242:TYR:HB2	4:B:610:HOH:O	2.19	0.43
1:C:324:CYS:HB3	1:C:328:GLN:O	2.19	0.42
1:D:190:LEU:HD12	1:D:190:LEU:HA	1.91	0.42
1:E:358:THR:O	3:G:2:IDS:O6A	2.37	0.42
1:C:64:LYS:HB3	2:H:2:IDS:H3	2.00	0.42
1:A:355:TYR:HE2	1:A:357:ASN:ND2	2.16	0.42
1:B:158:LEU:HB2	1:B:332:THR:HB	2.01	0.42
1:B:159:ILE:HG22	1:B:247:PHE:CE1	2.54	0.42
1:C:68:LEU:HG	1:C:336:THR:HG22	2.02	0.42
1:A:279:GLY:HA3	1:A:283:THR:O	2.19	0.42
1:D:237:MET:SD	1:D:246:LEU:HD23	2.58	0.42
1:E:335:ASP:OD1	1:E:337:THR:OG1	2.18	0.42
1:A:439:ASP:HA	1:A:440:PRO:HD2	1.93	0.42
1:A:131:ASN:ND2	1:E:128:ASP:OD2	2.43	0.42
1:B:163:PRO:HG3	1:B:441:LEU:CD2	2.50	0.42
1:B:237:MET:O	1:B:240:GLU:HB3	2.20	0.42
1:C:325:TRP:HB3	1:C:398:ILE:HD11	2.01	0.42
1:D:306:ILE:HD13	1:D:306:ILE:HA	1.59	0.42
1:A:161:CYS:SG	1:A:244:ASP:HB3	2.60	0.42
1:B:342:MET:HB2	1:C:208:MET:SD	2.60	0.42
1:A:54:LYS:HE2	1:A:55:PRO:HD2	2.01	0.42
1:B:120:HIS:HB2	1:B:221:PRO:HA	2.01	0.42
1:D:344:LEU:N	1:D:344:LEU:HD23	2.35	0.42
1:A:159:ILE:HG13	1:A:248:PHE:HD2	1.85	0.41
1:A:363:TYR:CD2	1:B:185:CYS:HB2	2.55	0.41
1:D:78:PRO:HD3	1:D:452:LYS:HA	2.02	0.41
1:B:54:LYS:H	1:B:54:LYS:HG3	1.59	0.41
1:C:37:ALA:HB1	1:C:451:LEU:HD13	2.02	0.41
1:A:52:ILE:HG12	1:B:269:GLU:CD	2.41	0.41
1:A:121:PRO:HG3	1:B:289:SER:HB3	2.03	0.41
1:A:151:TYR:CG	1:A:203:THR:HB	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASN:OD1	1:A:218:SER:HB2	2.20	0.41
1:D:126:LEU:HD13	1:D:264:ALA:HB2	2.02	0.41
1:B:74:ARG:HD3	1:B:76:HIS:CE1	2.56	0.41
1:A:43:LEU:HD12	1:A:43:LEU:HA	1.86	0.41
1:A:348:ILE:HG22	1:A:359:ASN:OD1	2.21	0.41
1:C:299:MET:HA	1:D:256:PHE:HB3	2.02	0.41
1:E:68:LEU:HD13	1:E:151:TYR:HD1	1.84	0.41
1:A:120:HIS:HB2	1:A:221:PRO:HA	2.02	0.41
1:A:178:VAL:HG23	1:A:179:ALA:O	2.20	0.41
1:C:105:VAL:HG21	1:C:159:ILE:HD13	2.03	0.41
1:C:126:LEU:HG	1:C:127:ASP:OD2	2.20	0.41
1:B:353:THR:O	1:D:278:LYS:HB2	2.20	0.41
1:A:109:ARG:HA	1:A:109:ARG:HD2	1.93	0.41
1:B:105:VAL:HG21	1:B:159:ILE:HD13	2.03	0.41
1:B:153:GLN:H	1:B:297:GLY:HA3	1.85	0.41
1:D:105:VAL:HG21	1:D:159:ILE:HD13	2.03	0.41
1:D:151:TYR:CG	1:D:203:THR:HB	2.56	0.41
1:A:324:CYS:HB3	1:A:328:GLN:O	2.20	0.41
1:B:78:PRO:HD3	1:B:452:LYS:HA	2.03	0.41
1:B:432:GLY:O	1:B:434:GLY:N	2.54	0.41
1:D:440:PRO:HG2	1:D:441:LEU:HD12	2.03	0.41
1:E:70:TYR:OH	1:E:232:PRO:HD3	2.21	0.41
1:E:175:CYS:C	1:E:177:ASN:H	2.21	0.41
1:E:235:ILE:H	1:E:235:ILE:HG12	1.63	0.41
1:B:201:VAL:O	1:B:203:THR:HG23	2.21	0.40
1:D:74:ARG:HB2	1:D:446:PHE:HB2	2.03	0.40
1:E:43:LEU:HD12	1:E:43:LEU:HA	1.91	0.40
1:E:237:MET:SD	1:E:246:LEU:HD23	2.61	0.40
1:A:366:HIS:HE2	1:A:368:GLU:CD	2.25	0.40
1:B:47:HIS:HB3	1:B:50:PHE:O	2.21	0.40
1:C:122:LEU:O	1:C:218:SER:HB3	2.20	0.40
1:D:34:TYR:HB2	1:D:459:LEU:HD11	2.03	0.40
1:B:48:PRO:HB3	1:B:341:ASN:ND2	2.35	0.40
1:D:111:GLN:HB3	1:D:112:PRO:HD2	2.04	0.40
1:B:112:PRO:HB3	1:C:231:TYR:CD1	2.56	0.40
1:C:74:ARG:NH2	1:C:439:ASP:OD2	2.54	0.40
1:E:121:PRO:HD3	1:E:222:LEU:HD21	2.02	0.40

All (13) 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:C:278:LYS:CE	2:J:2:IDS:O6B[2_545]	1.60	0.60
1:C:278:LYS:CE	2:J:2:IDS:O6A[2_545]	1.65	0.55
1:A:353:THR:CG2	2:J:2:IDS:O2S[2_545]	1.81	0.39
1:A:353:THR:OG1	2:J:2:IDS:O2[2_545]	1.81	0.39
1:C:278:LYS:CE	2:J:2:IDS:C6[2_545]	1.86	0.34
1:A:353:THR:OG1	2:J:2:IDS:O1S[2_545]	1.91	0.29
1:C:278:LYS:CG	2:J:2:IDS:O6A[2_545]	1.95	0.25
1:A:59:LYS:NZ	2:N:1:JHM:O1[2_546]	1.96	0.24
1:C:278:LYS:CB	2:J:2:IDS:O6A[2_545]	2.01	0.19
1:A:353:THR:OG1	2:J:2:IDS:S[2_545]	2.09	0.11
1:C:278:LYS:CD	2:J:2:IDS:O6A[2_545]	2.12	0.08
1:A:437:ALA:CB	3:G:6:IDS:O1S[2_546]	2.13	0.07
1:B:450:ASN:ND2	1:C:435:SER:O[2_645]	2.14	0.06

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	425/427 (100%)	391 (92%)	22 (5%)	12 (3%)	5	17
1	B	425/427 (100%)	384 (90%)	27 (6%)	14 (3%)	4	13
1	C	425/427 (100%)	390 (92%)	24 (6%)	11 (3%)	5	18
1	D	421/427 (99%)	388 (92%)	23 (6%)	10 (2%)	6	20
1	E	421/427 (99%)	386 (92%)	20 (5%)	15 (4%)	3	11
All	All	2117/2135 (99%)	1939 (92%)	116 (6%)	62 (3%)	4	15

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ALA
1	A	182	PRO
1	A	435	SER
1	A	437	ALA

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Mol	Chain	Res	Type
1	A	460	ASP
1	B	55	PRO
1	B	56	ASN
1	B	57	ASN
1	B	137	ALA
1	B	403	ASN
1	C	137	ALA
1	C	433	GLY
1	C	437	ALA
1	D	137	ALA
1	D	176	THR
1	D	298	SER
1	D	403	ASN
1	D	437	ALA
1	E	137	ALA
1	E	176	THR
1	E	352	GLU
1	E	353	THR
1	E	402	TRP
1	E	435	SER
1	E	437	ALA
1	A	41	ARG
1	A	403	ASN
1	B	126	LEU
1	B	142	ASP
1	B	298	SER
1	B	434	GLY
1	C	435	SER
1	C	460	ASP
1	D	434	GLY
1	E	58	ASN
1	E	395	ASN
1	A	142	ASP
1	A	176	THR
1	B	40	SER
1	B	216	ASN
1	C	41	ARG
1	C	298	SER
1	C	402	TRP
1	D	142	ASP
1	A	126	LEU
1	A	298	SER

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Mol	Chain	Res	Type
1	B	396	SER
1	C	126	LEU
1	C	176	THR
1	D	216	ASN
1	E	142	ASP
1	E	248	PHE
1	A	174	PRO
1	B	54	LYS
1	D	472	ALA
1	E	126	LEU
1	E	298	SER
1	E	350	THR
1	E	131	ASN
1	B	433	GLY
1	C	473	GLY
1	D	93	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	368/368 (100%)	326 (89%)	42 (11%)	5 18
1	B	368/368 (100%)	337 (92%)	31 (8%)	11 31
1	C	368/368 (100%)	330 (90%)	38 (10%)	7 21
1	D	366/368 (100%)	334 (91%)	32 (9%)	10 30
1	E	366/368 (100%)	329 (90%)	37 (10%)	7 22
All	All	1836/1840 (100%)	1656 (90%)	180 (10%)	8 24

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	54	LYS
1	A	60	ILE

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Mol	Chain	Res	Type
1	A	68	LEU
1	A	74	ARG
1	A	96	GLN
1	A	99	VAL
1	A	106	GLU
1	A	122	LEU
1	A	127	ASP
1	A	159	ILE
1	A	177	ASN
1	A	180	VAL
1	A	193	THR
1	A	201	VAL
1	A	213	LEU
1	A	222	LEU
1	A	225	CYS
1	A	245	SER
1	A	251	ARG
1	A	273	ASP
1	A	286	LEU
1	A	294	THR
1	A	301	THR
1	A	302	SER
1	A	306	ILE
1	A	313	LEU
1	A	315	ARG
1	A	317	GLN
1	A	329	LEU
1	A	342	MET
1	A	344	LEU
1	A	348	ILE
1	A	352	GLU
1	A	358	THR
1	A	380	LYS
1	A	391	ILE
1	A	397	THR
1	A	438	GLU
1	A	442	LYS
1	A	453	GLU
1	A	464	LEU
1	B	54	LYS
1	B	56	ASN
1	B	60	ILE

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Mol	Chain	Res	Type
1	B	68	LEU
1	B	74	ARG
1	B	91	TYR
1	B	94	ASP
1	B	95	THR
1	B	106	GLU
1	B	127	ASP
1	B	178	VAL
1	B	188	LEU
1	B	193	THR
1	B	213	LEU
1	B	222	LEU
1	B	247	PHE
1	B	251	ARG
1	B	262	ASN
1	B	286	LEU
1	B	294	THR
1	B	301	THR
1	B	306	ILE
1	B	315	ARG
1	B	317	GLN
1	B	329	LEU
1	B	344	LEU
1	B	345	CYS
1	B	352	GLU
1	B	368	GLU
1	B	380	LYS
1	B	464	LEU
1	C	56	ASN
1	C	60	ILE
1	C	66	SER
1	C	68	LEU
1	C	74	ARG
1	C	94	ASP
1	C	96	GLN
1	C	106	GLU
1	C	117	ILE
1	C	127	ASP
1	C	133	SER
1	C	141	VAL
1	C	175	CYS
1	C	177	ASN

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Mol	Chain	Res	Type
1	C	193	THR
1	C	201	VAL
1	C	213	LEU
1	C	222	LEU
1	C	247	PHE
1	C	251	ARG
1	C	262	ASN
1	C	270	ASN
1	C	273	ASP
1	C	301	THR
1	C	306	ILE
1	C	315	ARG
1	C	317	GLN
1	C	329	LEU
1	C	342	MET
1	C	344	LEU
1	C	348	ILE
1	C	351	SER
1	C	352	GLU
1	C	438	GLU
1	C	442	LYS
1	C	443	LYS
1	C	453	GLU
1	C	464	LEU
1	D	59	LYS
1	D	60	ILE
1	D	74	ARG
1	D	88	THR
1	D	91	TYR
1	D	95	THR
1	D	96	GLN
1	D	106	GLU
1	D	117	ILE
1	D	127	ASP
1	D	175	CYS
1	D	178	VAL
1	D	193	THR
1	D	195	ILE
1	D	201	VAL
1	D	213	LEU
1	D	222	LEU
1	D	225	CYS

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Mol	Chain	Res	Type
1	D	245	SER
1	D	251	ARG
1	D	273	ASP
1	D	286	LEU
1	D	294	THR
1	D	301	THR
1	D	306	ILE
1	D	315	ARG
1	D	317	GLN
1	D	329	LEU
1	D	344	LEU
1	D	352	GLU
1	D	453	GLU
1	D	464	LEU
1	E	43	LEU
1	E	58	ASN
1	E	60	ILE
1	E	66	SER
1	E	68	LEU
1	E	74	ARG
1	E	82	LYS
1	E	96	GLN
1	E	106	GLU
1	E	127	ASP
1	E	138	ASN
1	E	176	THR
1	E	178	VAL
1	E	188	LEU
1	E	213	LEU
1	E	222	LEU
1	E	225	CYS
1	E	246	LEU
1	E	251	ARG
1	E	294	THR
1	E	301	THR
1	E	306	ILE
1	E	314	GLN
1	E	315	ARG
1	E	317	GLN
1	E	329	LEU
1	E	342	MET
1	E	344	LEU

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Mol	Chain	Res	Type
1	E	345	CYS
1	E	350	THR
1	E	356	LYS
1	E	386	ASP
1	E	396	SER
1	E	453	GLU
1	E	460	ASP
1	E	464	LEU
1	E	470	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	357	ASN
1	B	341	ASN
1	C	96	GLN
1	C	196	GLN
1	C	319	HIS
1	C	341	ASN
1	C	366	HIS
1	D	192	ASN
1	E	319	HIS
1	E	341	ASN
1	E	357	ASN
1	E	366	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)

26 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	$\#\|Z\| > 2$
2	JHM	F	1	2	15,15,15	1.08	2 (13%)	18,22,22	1.25	2 (11%)
2	IDS	F	2	2	15,15,17	1.96	1 (6%)	15,22,26	2.34	4 (26%)
3	JHM	G	1	3	15,15,15	1.09	2 (13%)	18,22,22	1.24	2 (11%)
3	IDS	G	2	3	16,16,17	1.95	2 (12%)	17,24,26	2.18	3 (17%)
3	JHM	G	3	3	14,14,15	0.96	1 (7%)	18,20,22	1.44	3 (16%)
3	IDS	G	4	3	16,16,17	1.94	2 (12%)	17,24,26	4.47	6 (35%)
3	JHM	G	5	3	14,14,15	0.96	1 (7%)	18,20,22	1.43	3 (16%)
3	IDS	G	6	3	15,15,17	1.96	2 (13%)	15,22,26	2.35	4 (26%)
2	JHM	H	1	2	15,15,15	1.09	2 (13%)	18,22,22	1.27	2 (11%)
2	IDS	H	2	2	15,15,17	1.97	2 (13%)	15,22,26	2.34	4 (26%)
2	JHM	I	1	2	15,15,15	1.09	2 (13%)	18,22,22	1.27	2 (11%)
2	IDS	I	2	2	15,15,17	1.94	1 (6%)	15,22,26	2.32	4 (26%)
2	JHM	J	1	2	15,15,15	1.08	2 (13%)	18,22,22	1.26	2 (11%)
2	IDS	J	2	2,1	15,15,17	1.95	1 (6%)	15,22,26	2.32	4 (26%)
2	JHM	K	1	2	15,15,15	1.09	2 (13%)	18,22,22	1.25	2 (11%)
2	IDS	K	2	2	15,15,17	1.94	1 (6%)	15,22,26	2.32	4 (26%)
2	JHM	L	1	2	15,15,15	1.08	2 (13%)	18,22,22	1.26	2 (11%)
2	IDS	L	2	2	15,15,17	1.98	2 (13%)	15,22,26	2.34	4 (26%)
2	JHM	M	1	2	15,15,15	1.07	2 (13%)	18,22,22	1.26	2 (11%)
2	IDS	M	2	2	15,15,17	1.96	2 (13%)	15,22,26	2.33	4 (26%)
2	JHM	N	1	2	15,15,15	1.07	2 (13%)	18,22,22	1.25	2 (11%)
2	IDS	N	2	2	15,15,17	1.95	1 (6%)	15,22,26	2.33	4 (26%)
2	JHM	O	1	2	15,15,15	1.07	2 (13%)	18,22,22	1.24	2 (11%)
2	IDS	O	2	2	15,15,17	1.95	1 (6%)	15,22,26	2.33	4 (26%)
2	JHM	P	1	2	15,15,15	1.08	2 (13%)	18,22,22	1.26	2 (11%)
2	IDS	P	2	2	15,15,17	1.94	1 (6%)	15,22,26	2.32	4 (26%)

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
2	JHM	F	1	2	-	2/6/22/22	0/1/1/1
2	IDS	F	2	2	-	1/9/22/29	0/1/1/1
3	JHM	G	1	3	-	2/6/22/22	0/1/1/1
3	IDS	G	2	3	-	0/9/26/29	0/1/1/1
3	JHM	G	3	3	-	0/6/20/22	0/1/1/1
3	IDS	G	4	3	-	0/9/26/29	0/1/1/1
3	JHM	G	5	3	-	0/6/20/22	0/1/1/1
3	IDS	G	6	3	-	0/9/22/29	0/1/1/1
2	JHM	H	1	2	-	0/6/22/22	0/1/1/1
2	IDS	H	2	2	-	0/9/22/29	0/1/1/1
2	JHM	I	1	2	-	0/6/22/22	0/1/1/1
2	IDS	I	2	2	-	1/9/22/29	0/1/1/1
2	JHM	J	1	2	-	2/6/22/22	0/1/1/1
2	IDS	J	2	2,1	-	1/9/22/29	0/1/1/1
2	JHM	K	1	2	-	2/6/22/22	0/1/1/1
2	IDS	K	2	2	-	1/9/22/29	0/1/1/1
2	JHM	L	1	2	-	1/6/22/22	0/1/1/1
2	IDS	L	2	2	-	0/9/22/29	0/1/1/1
2	JHM	M	1	2	-	1/6/22/22	0/1/1/1
2	IDS	M	2	2	-	0/9/22/29	0/1/1/1
2	JHM	N	1	2	-	2/6/22/22	0/1/1/1
2	IDS	N	2	2	-	1/9/22/29	0/1/1/1
2	JHM	O	1	2	-	2/6/22/22	0/1/1/1
2	IDS	O	2	2	-	1/9/22/29	0/1/1/1
2	JHM	P	1	2	-	1/6/22/22	0/1/1/1
2	IDS	P	2	2	-	1/9/22/29	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	IDS	O2-C2	-6.57	1.37	1.47
2	N	2	IDS	O2-C2	-6.56	1.37	1.47
2	L	2	IDS	O2-C2	-6.54	1.37	1.47
2	J	2	IDS	O2-C2	-6.53	1.37	1.47
2	O	2	IDS	O2-C2	-6.52	1.37	1.47
3	G	4	IDS	O2-C2	-6.51	1.37	1.47
2	H	2	IDS	O2-C2	-6.50	1.37	1.47
2	P	2	IDS	O2-C2	-6.49	1.37	1.47
3	G	6	IDS	O2-C2	-6.49	1.37	1.47
2	I	2	IDS	O2-C2	-6.48	1.37	1.47
2	K	2	IDS	O2-C2	-6.47	1.37	1.47
3	G	2	IDS	O2-C2	-6.46	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	2	IDS	O2-C2	-6.45	1.37	1.47
3	G	2	IDS	O4-C4	-2.25	1.37	1.43
2	I	1	JHM	C3-C4	2.24	1.55	1.52
2	H	1	JHM	O1-C1	2.21	1.45	1.39
2	M	2	IDS	O6B-C6	-2.21	1.23	1.30
2	K	1	JHM	O1-C1	2.20	1.45	1.39
2	F	1	JHM	O1-C1	2.20	1.45	1.39
3	G	4	IDS	O6B-C6	-2.20	1.23	1.30
3	G	1	JHM	O1-C1	2.19	1.45	1.39
2	M	1	JHM	O1-C1	2.19	1.45	1.39
3	G	6	IDS	O6B-C6	-2.18	1.23	1.30
2	J	1	JHM	C3-C4	2.18	1.55	1.52
2	N	1	JHM	O1-C1	2.18	1.45	1.39
2	K	1	JHM	C3-C4	2.18	1.55	1.52
2	I	1	JHM	O1-C1	2.17	1.45	1.39
2	L	2	IDS	O6B-C6	-2.17	1.23	1.30
2	L	1	JHM	O1-C1	2.16	1.45	1.39
2	O	1	JHM	O1-C1	2.16	1.45	1.39
2	H	2	IDS	O6B-C6	-2.16	1.23	1.30
2	J	1	JHM	O1-C1	2.14	1.45	1.39
2	L	1	JHM	C3-C4	2.13	1.55	1.52
2	H	1	JHM	C3-C4	2.13	1.55	1.52
2	P	1	JHM	O1-C1	2.13	1.45	1.39
3	G	3	JHM	C3-C4	2.12	1.55	1.52
3	G	1	JHM	C3-C4	2.11	1.55	1.52
2	P	1	JHM	C3-C4	2.11	1.55	1.52
2	N	1	JHM	C3-C4	2.08	1.55	1.52
2	O	1	JHM	C3-C4	2.07	1.55	1.52
3	G	5	JHM	C3-C4	2.06	1.55	1.52
2	M	1	JHM	C3-C4	2.06	1.55	1.52
2	F	1	JHM	C3-C4	2.01	1.55	1.52

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	4	IDS	O4-C4-C5	15.51	144.52	109.74
2	F	2	IDS	C2-O2-S	7.13	127.20	117.91
2	P	2	IDS	C2-O2-S	7.12	127.20	117.91
2	O	2	IDS	C2-O2-S	7.11	127.19	117.91
2	N	2	IDS	C2-O2-S	7.09	127.16	117.91
3	G	2	IDS	C2-O2-S	7.09	127.15	117.91
3	G	4	IDS	C2-O2-S	7.08	127.15	117.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	2	IDS	C2-O2-S	7.08	127.15	117.91
2	H	2	IDS	C2-O2-S	7.07	127.13	117.91
3	G	6	IDS	C2-O2-S	7.06	127.12	117.91
2	J	2	IDS	C2-O2-S	7.06	127.12	117.91
2	K	2	IDS	C2-O2-S	7.05	127.11	117.91
2	I	2	IDS	C2-O2-S	7.05	127.10	117.91
2	M	2	IDS	C2-O2-S	7.04	127.09	117.91
3	G	4	IDS	O4-C4-C3	-4.35	100.30	110.35
3	G	3	JHM	C2-C3-C4	-3.49	107.14	111.16
3	G	5	JHM	C2-C3-C4	-3.45	107.20	111.16
2	J	1	JHM	C3-C4-C5	-3.36	106.62	109.97
2	N	1	JHM	C3-C4-C5	-3.32	106.66	109.97
2	I	1	JHM	C3-C4-C5	-3.32	106.67	109.97
2	L	1	JHM	C3-C4-C5	-3.30	106.68	109.97
2	H	1	JHM	C3-C4-C5	-3.30	106.68	109.97
2	K	1	JHM	C3-C4-C5	-3.29	106.69	109.97
2	F	1	JHM	C3-C4-C5	-3.29	106.69	109.97
3	G	3	JHM	C3-C4-C5	-3.28	106.71	109.97
3	G	5	JHM	C3-C4-C5	-3.27	106.71	109.97
3	G	1	JHM	C3-C4-C5	-3.25	106.73	109.97
2	P	1	JHM	C3-C4-C5	-3.25	106.73	109.97
2	O	1	JHM	C3-C4-C5	-3.24	106.74	109.97
2	M	1	JHM	C3-C4-C5	-3.23	106.75	109.97
3	G	4	IDS	C1-C2-C3	2.93	113.78	109.40
3	G	2	IDS	C1-C2-C3	2.92	113.76	109.40
3	G	6	IDS	O6B-C6-C5	2.80	121.01	113.03
2	M	2	IDS	O6B-C6-C5	2.78	120.97	113.03
2	L	2	IDS	O6B-C6-C5	2.77	120.94	113.03
2	H	2	IDS	O6B-C6-C5	2.77	120.94	113.03
2	P	2	IDS	C1-C2-C3	2.74	113.82	109.94
2	O	2	IDS	C1-C2-C3	2.73	113.81	109.94
2	N	2	IDS	C1-C2-C3	2.71	113.78	109.94
2	L	2	IDS	C1-C2-C3	2.71	113.78	109.94
3	G	6	IDS	C1-C2-C3	2.69	113.75	109.94
2	M	2	IDS	C1-C2-C3	2.69	113.74	109.94
2	K	2	IDS	C1-C2-C3	2.68	113.74	109.94
2	I	2	IDS	C1-C2-C3	2.68	113.73	109.94
2	H	2	IDS	C1-C2-C3	2.65	113.69	109.94
2	J	2	IDS	C1-C2-C3	2.63	113.66	109.94
2	F	2	IDS	C1-C2-C3	2.63	113.66	109.94
2	F	2	IDS	O6B-C6-C5	2.57	120.36	113.03
2	N	2	IDS	O6B-C6-C5	2.55	120.31	113.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	2	IDS	O6B-C6-C5	2.54	120.29	113.03
2	O	2	IDS	O6B-C6-C5	2.54	120.27	113.03
2	P	2	IDS	O6B-C6-C5	2.53	120.26	113.03
2	J	2	IDS	O6B-C6-C5	2.53	120.25	113.03
2	K	2	IDS	O6B-C6-C5	2.53	120.25	113.03
2	M	1	JHM	C2-C3-C4	-2.43	107.16	110.69
2	I	1	JHM	C2-C3-C4	-2.42	107.17	110.69
2	K	1	JHM	C2-C3-C4	-2.42	107.17	110.69
3	G	1	JHM	C2-C3-C4	-2.41	107.19	110.69
2	H	1	JHM	C2-C3-C4	-2.40	107.20	110.69
2	N	1	JHM	C2-C3-C4	-2.40	107.20	110.69
2	P	1	JHM	C2-C3-C4	-2.39	107.21	110.69
2	F	2	IDS	O6B-C6-O6A	-2.39	118.66	124.09
2	F	1	JHM	C2-C3-C4	-2.39	107.22	110.69
2	O	1	JHM	C2-C3-C4	-2.38	107.22	110.69
3	G	4	IDS	O6B-C6-O6A	-2.38	118.68	124.09
2	L	1	JHM	C2-C3-C4	-2.38	107.22	110.69
2	J	2	IDS	O6B-C6-O6A	-2.38	118.69	124.09
2	J	1	JHM	C2-C3-C4	-2.38	107.23	110.69
3	G	2	IDS	O6B-C6-O6A	-2.37	118.70	124.09
2	N	2	IDS	O6B-C6-O6A	-2.36	118.73	124.09
3	G	6	IDS	O6B-C6-O6A	-2.36	118.74	124.09
2	P	2	IDS	O6B-C6-O6A	-2.35	118.75	124.09
2	K	2	IDS	O6B-C6-O6A	-2.34	118.77	124.09
2	L	2	IDS	O6B-C6-O6A	-2.34	118.77	124.09
2	I	2	IDS	O6B-C6-O6A	-2.34	118.78	124.09
2	M	2	IDS	O6B-C6-O6A	-2.33	118.79	124.09
2	O	2	IDS	O6B-C6-O6A	-2.33	118.79	124.09
2	H	2	IDS	O6B-C6-O6A	-2.33	118.81	124.09
3	G	5	JHM	C1-C2-C3	-2.20	107.00	110.68
3	G	3	JHM	C1-C2-C3	-2.20	107.01	110.68
3	G	4	IDS	O6B-C6-C5	2.02	121.04	113.65

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	JHM	C6-O6-S-O8
2	J	1	JHM	C6-O6-S-O8
2	K	1	JHM	C6-O6-S-O8
2	N	1	JHM	C6-O6-S-O8
2	O	1	JHM	C6-O6-S-O8

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Mol	Chain	Res	Type	Atoms
3	G	1	JHM	C6-O6-S-O8
2	F	1	JHM	C6-O6-S-O9
2	J	1	JHM	C6-O6-S-O9
2	K	1	JHM	C6-O6-S-O9
2	L	1	JHM	C6-O6-S-O7
2	M	1	JHM	C6-O6-S-O7
2	N	1	JHM	C6-O6-S-O9
2	O	1	JHM	C6-O6-S-O9
2	P	1	JHM	C6-O6-S-O7
3	G	1	JHM	C6-O6-S-O9
2	F	2	IDS	C4-C5-C6-O6A
2	I	2	IDS	C4-C5-C6-O6A
2	J	2	IDS	C4-C5-C6-O6A
2	K	2	IDS	C4-C5-C6-O6A
2	N	2	IDS	C4-C5-C6-O6A
2	O	2	IDS	C4-C5-C6-O6A
2	P	2	IDS	C4-C5-C6-O6A

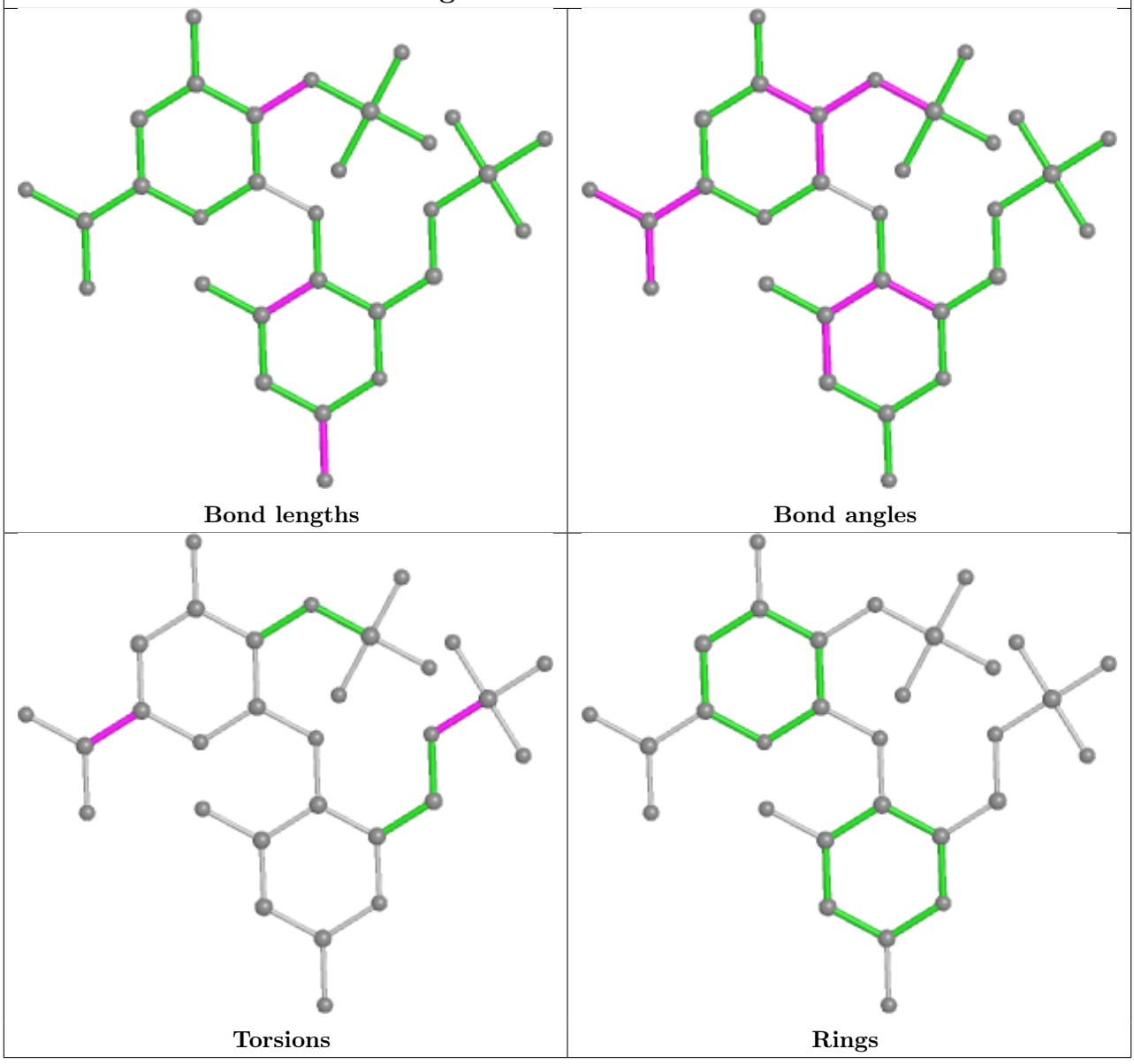
There are no ring outliers.

19 monomers are involved in 106 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	3	JHM	2	0
2	H	1	JHM	9	0
2	K	1	JHM	5	0
2	H	2	IDS	4	0
2	J	2	IDS	2	10
2	I	1	JHM	6	0
2	N	1	JHM	4	1
2	O	1	JHM	4	0
2	F	1	JHM	22	0
2	I	2	IDS	10	0
3	G	2	IDS	5	0
2	M	1	JHM	6	0
2	J	1	JHM	10	0
3	G	6	IDS	0	1
2	P	1	JHM	8	0
2	P	2	IDS	4	0
3	G	1	JHM	4	0
2	O	2	IDS	4	0
2	L	2	IDS	5	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.

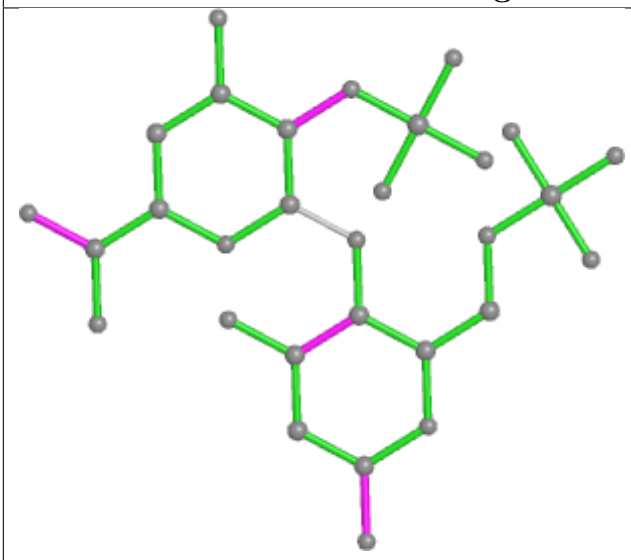
Oligosaccharide Chain F



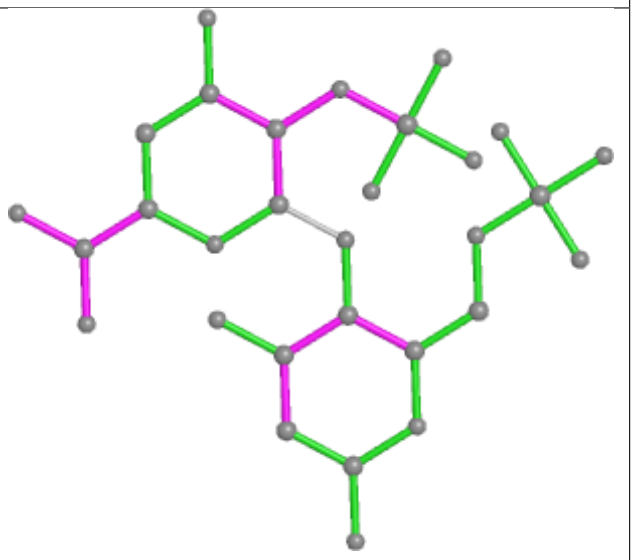
Bond lengths | **Bond angles**

Torsions | **Rings**

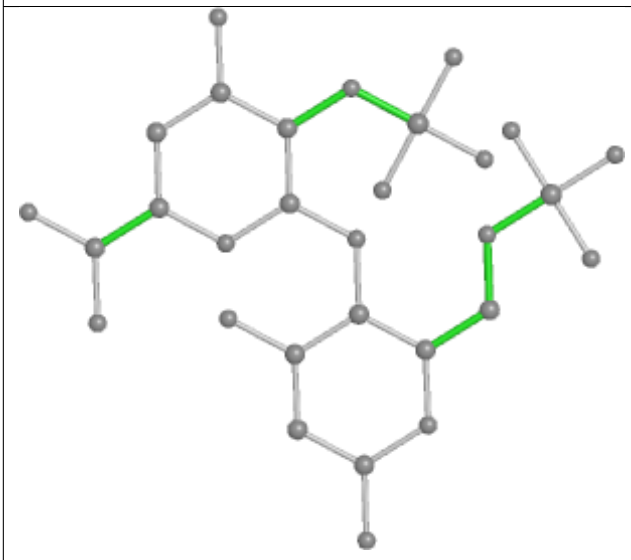
Oligosaccharide Chain H



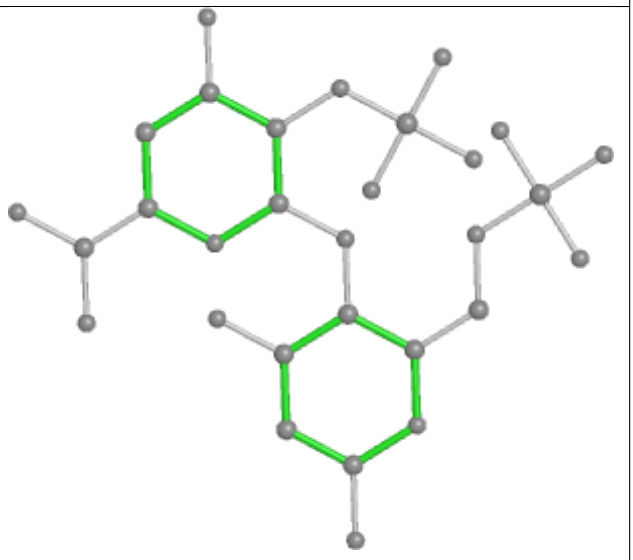
Bond lengths



Bond angles

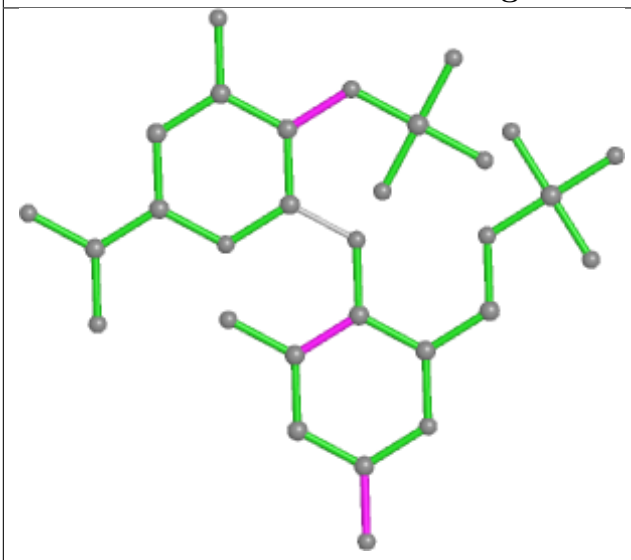


Torsions

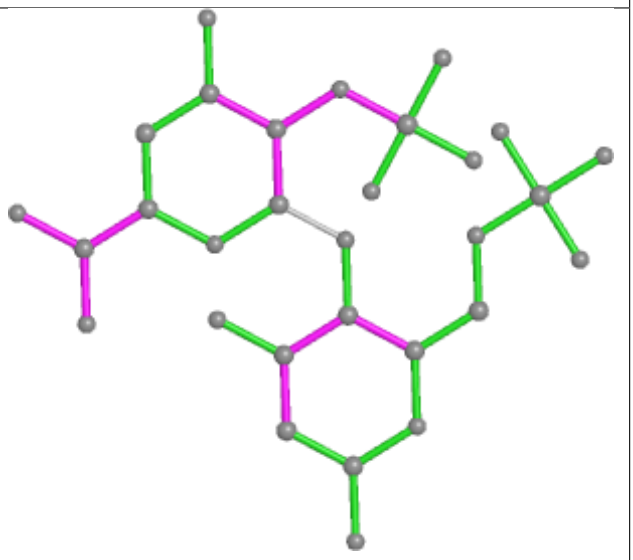


Rings

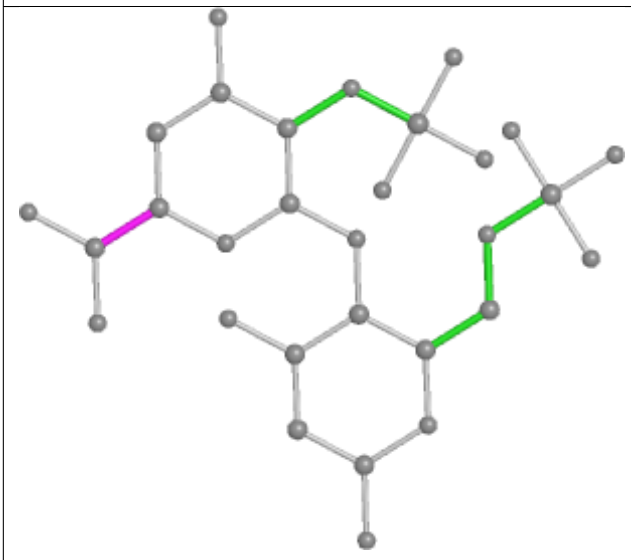
Oligosaccharide Chain I



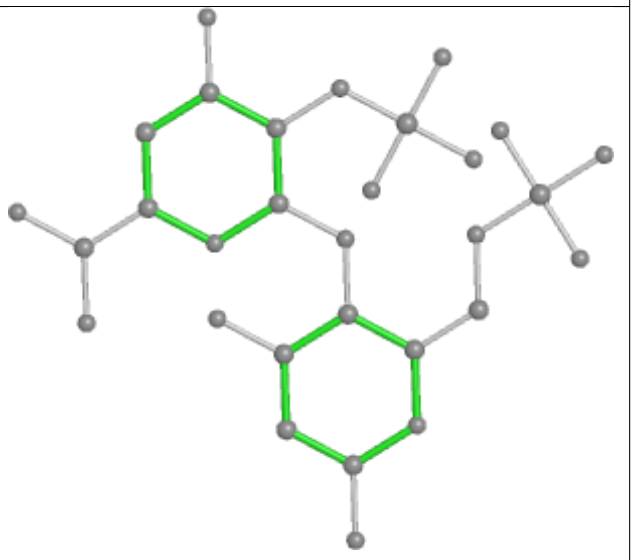
Bond lengths



Bond angles

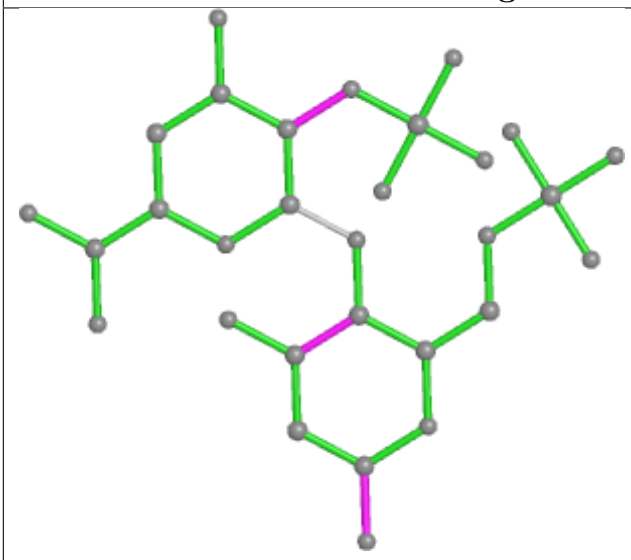


Torsions

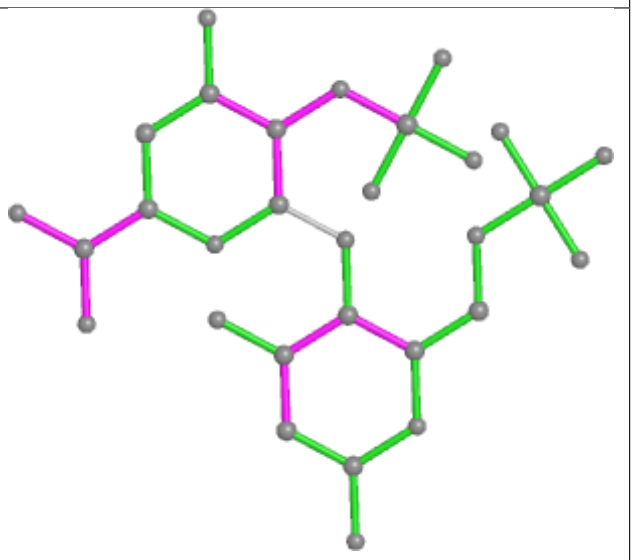


Rings

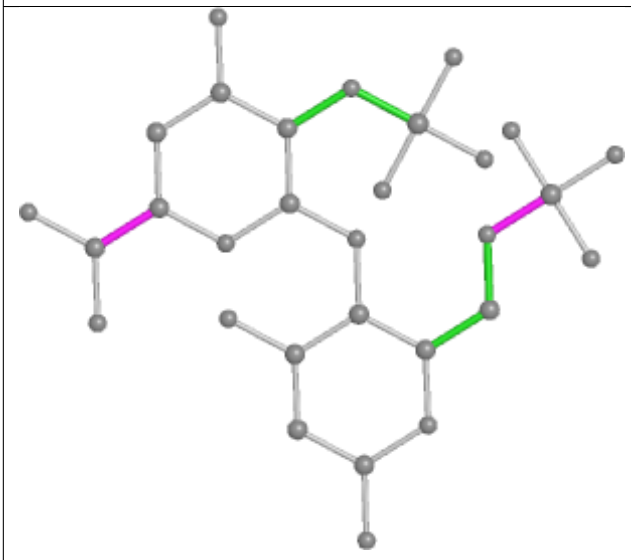
Oligosaccharide Chain J



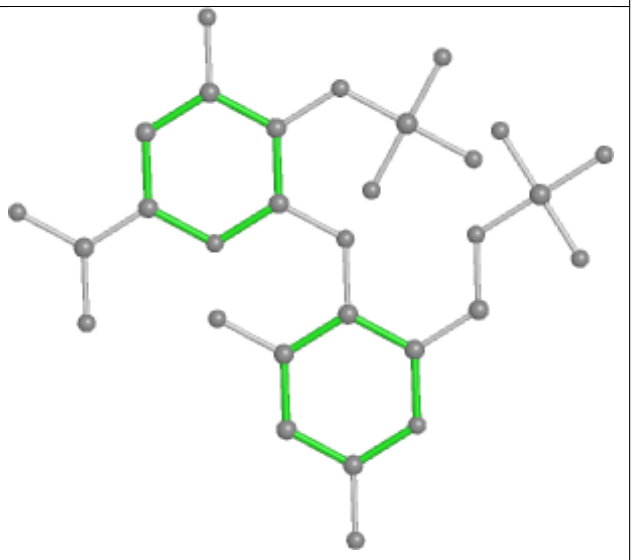
Bond lengths



Bond angles

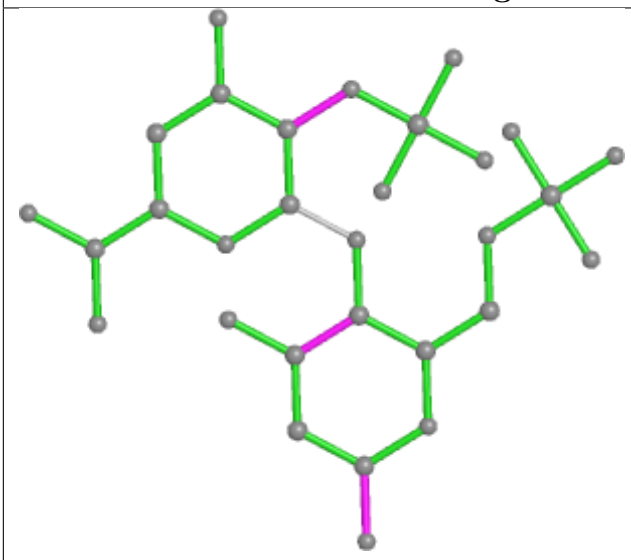


Torsions

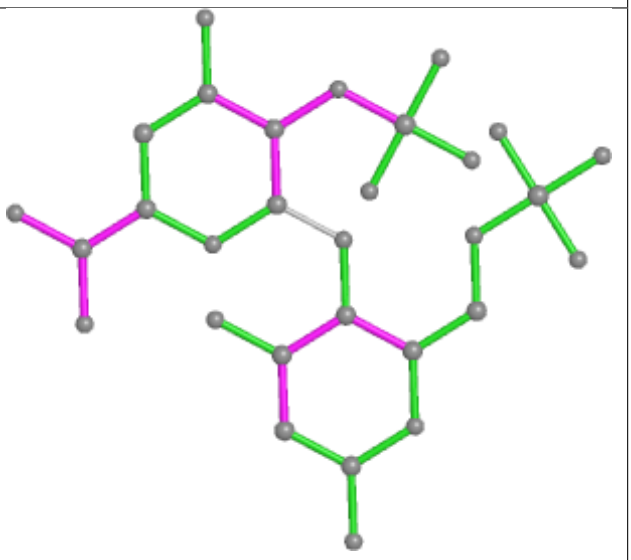


Rings

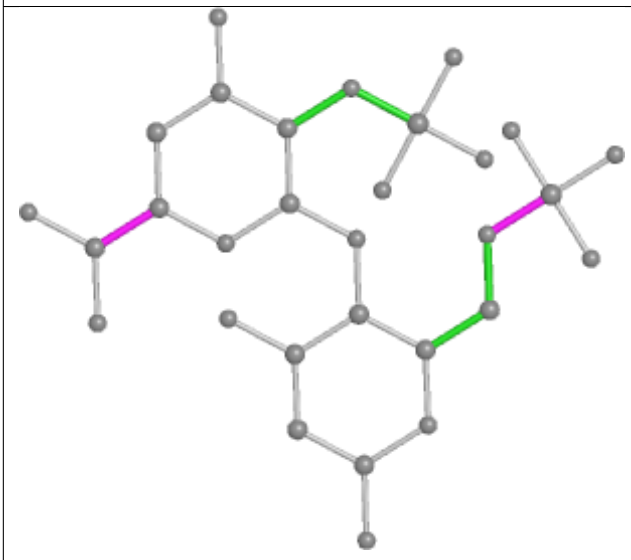
Oligosaccharide Chain K



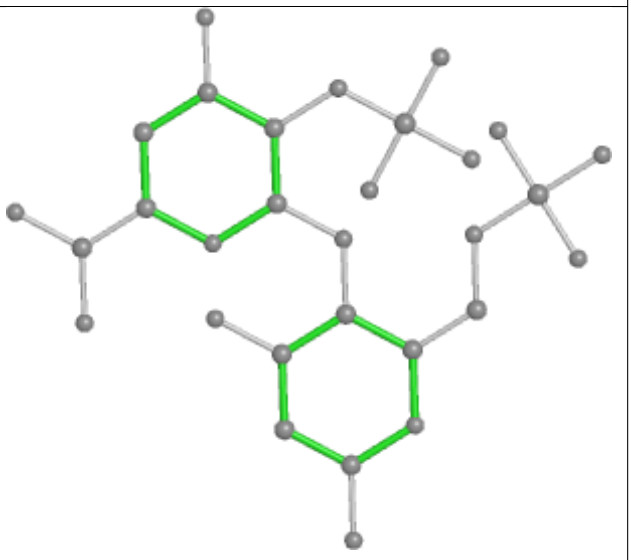
Bond lengths



Bond angles

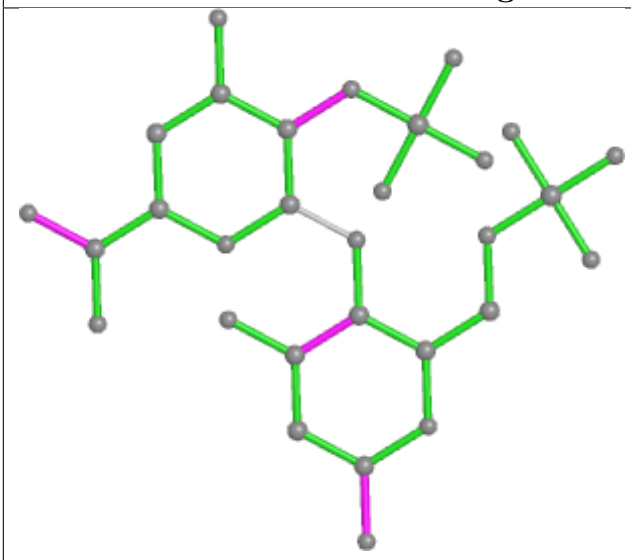


Torsions

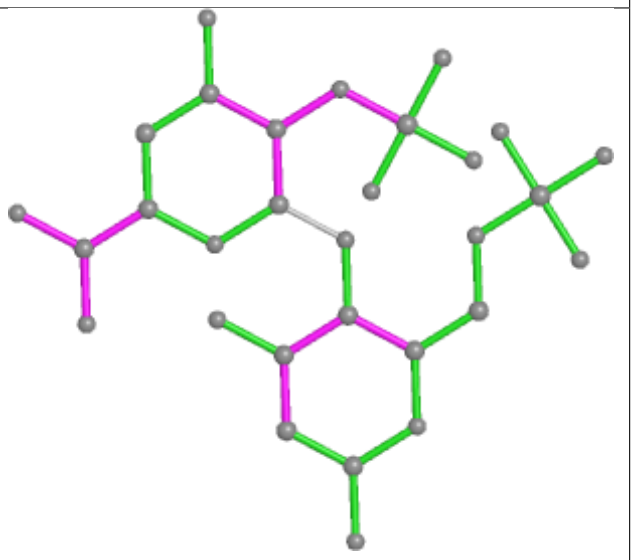


Rings

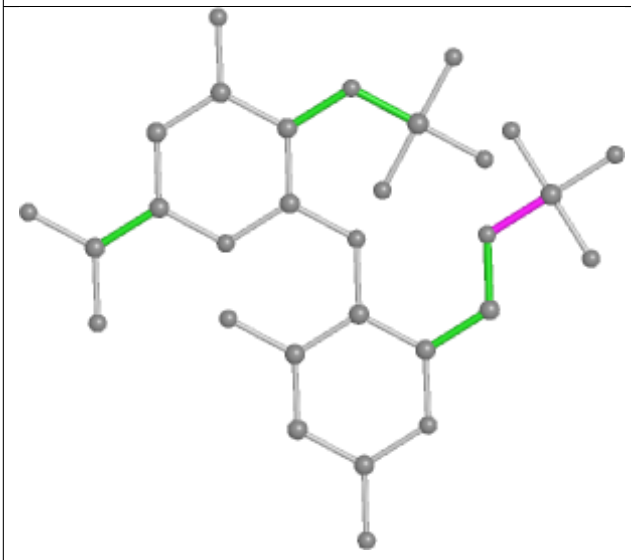
Oligosaccharide Chain L



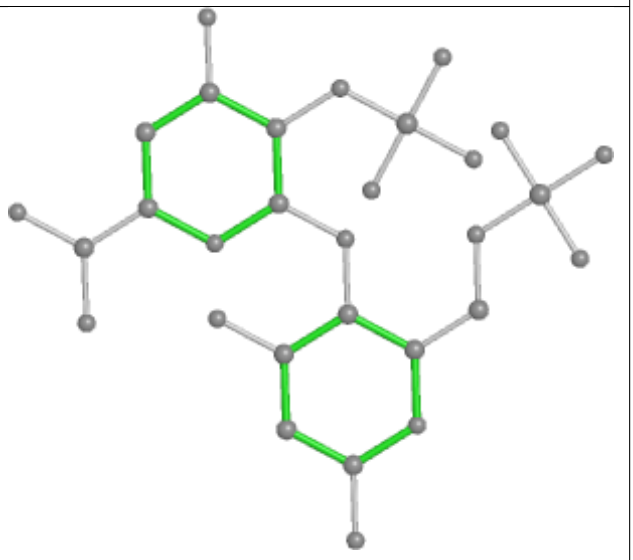
Bond lengths



Bond angles

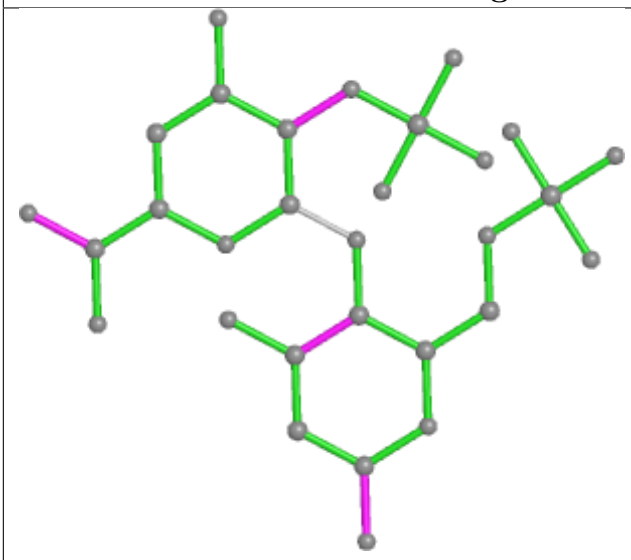


Torsions

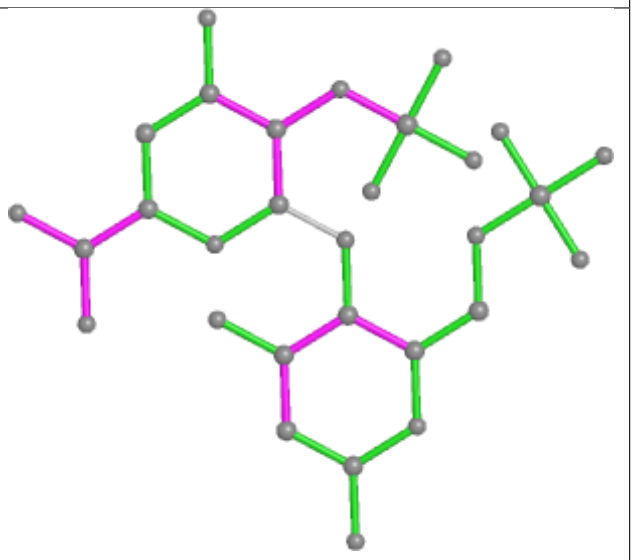


Rings

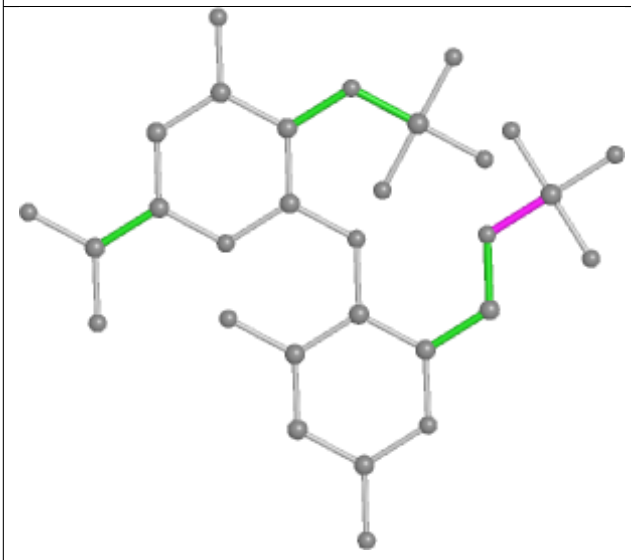
Oligosaccharide Chain M



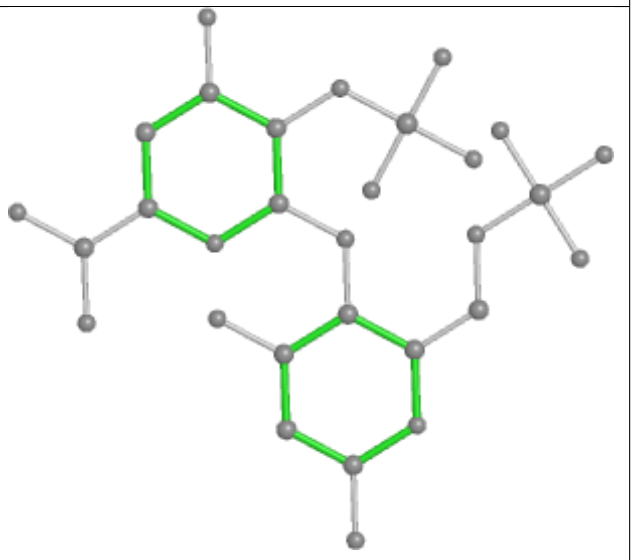
Bond lengths



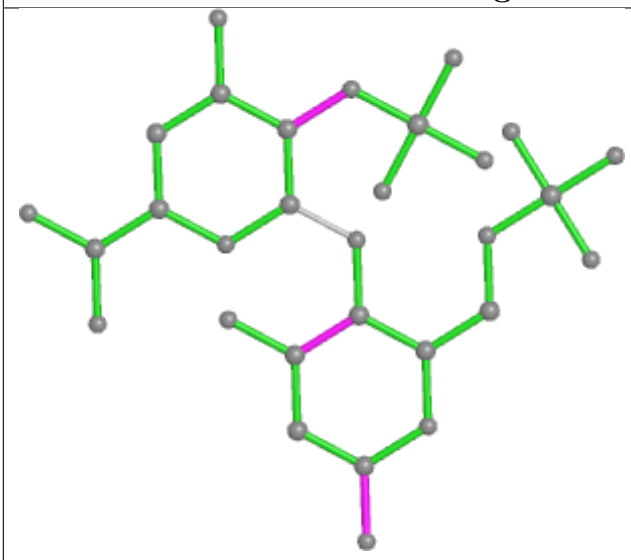
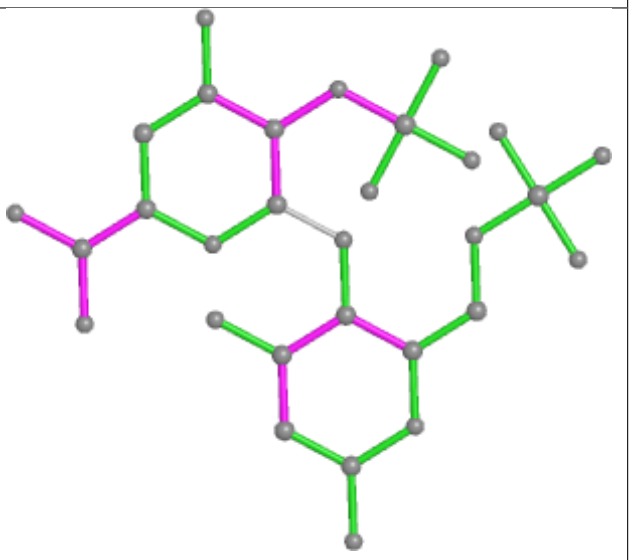
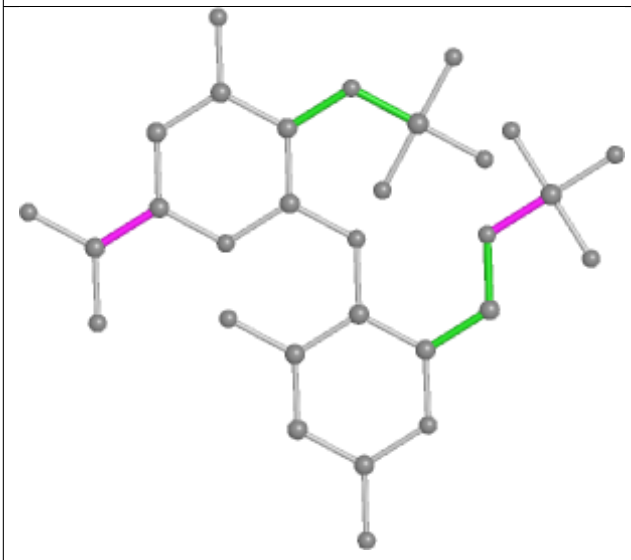
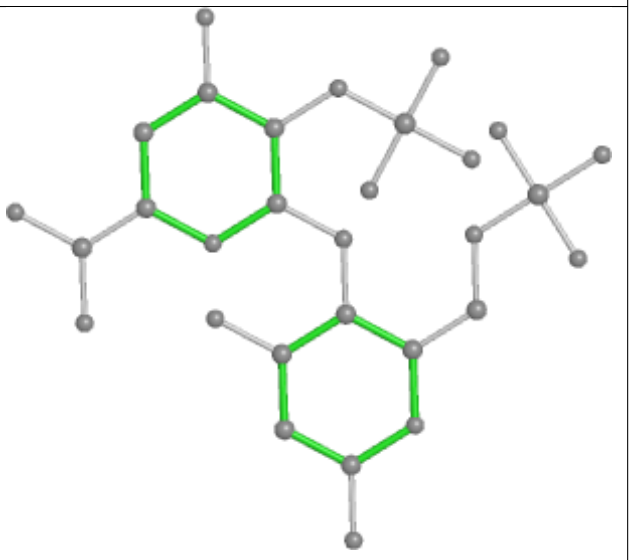
Bond angles



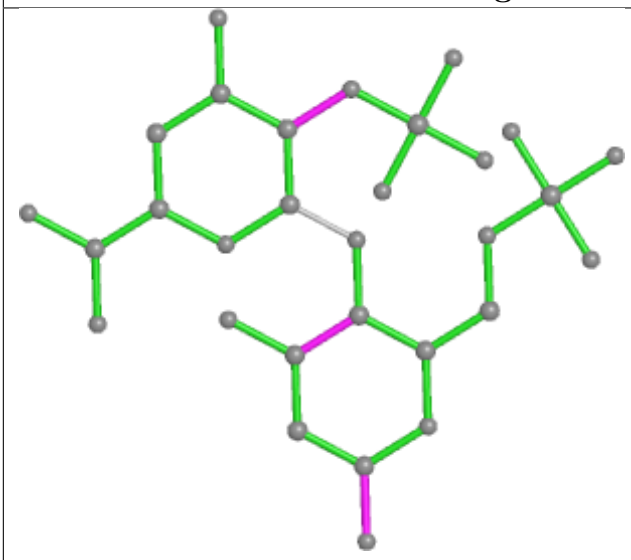
Torsions



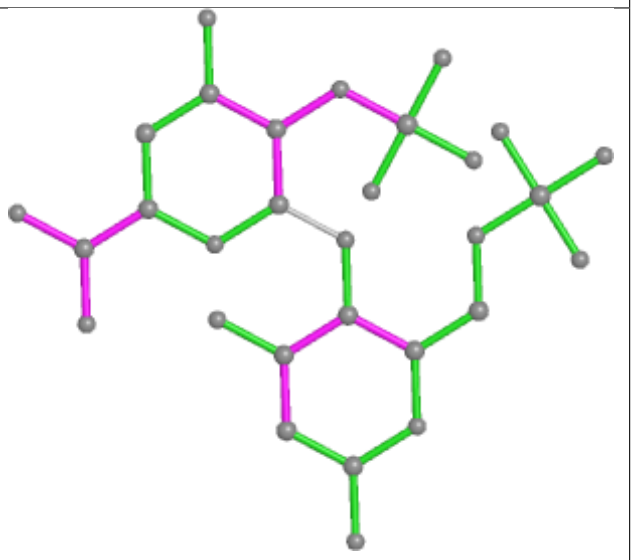
Rings

Oligosaccharide Chain N	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

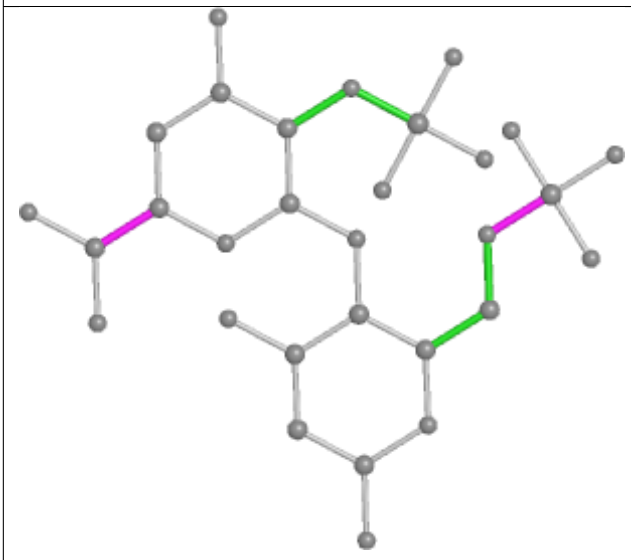
Oligosaccharide Chain O



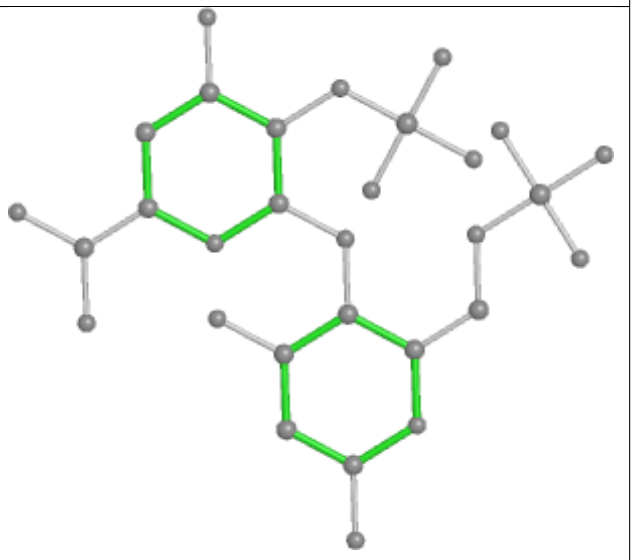
Bond lengths



Bond angles

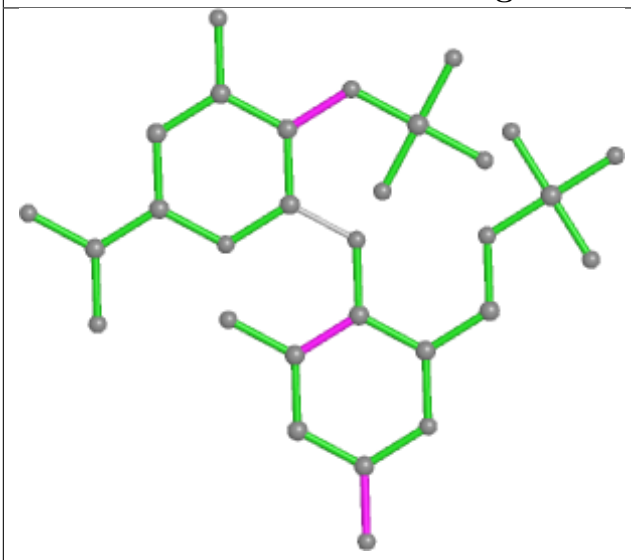


Torsions

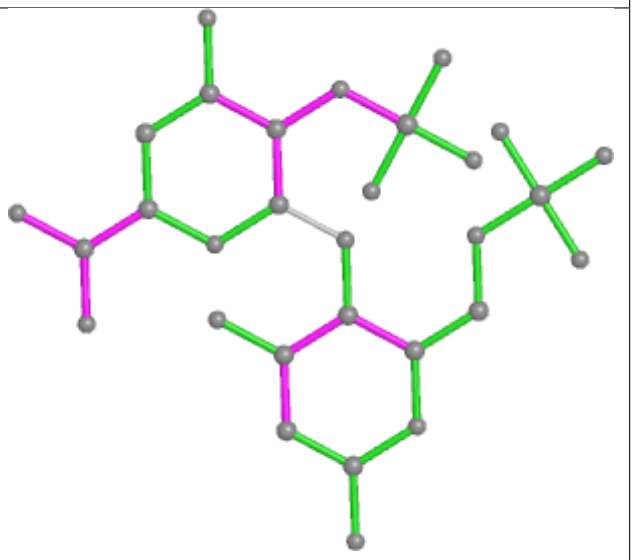


Rings

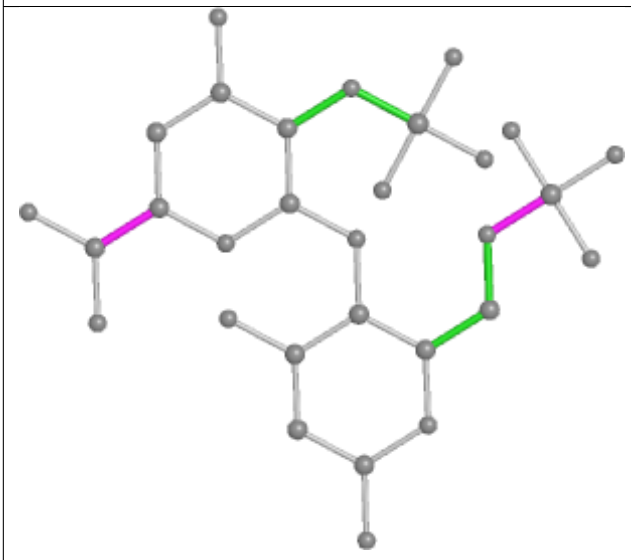
Oligosaccharide Chain P



Bond lengths



Bond angles



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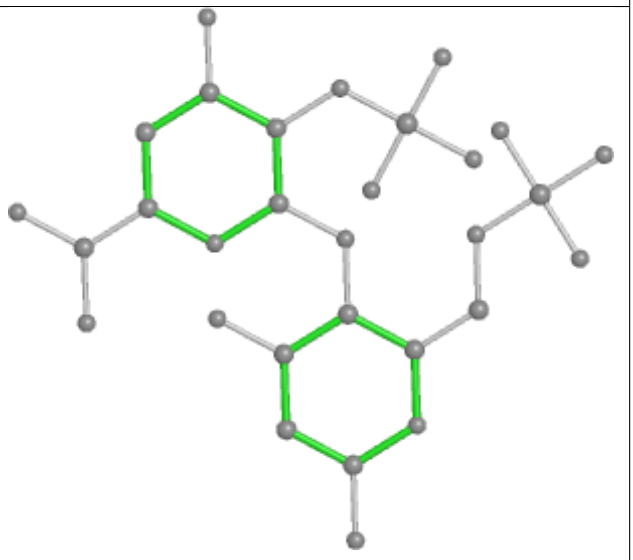
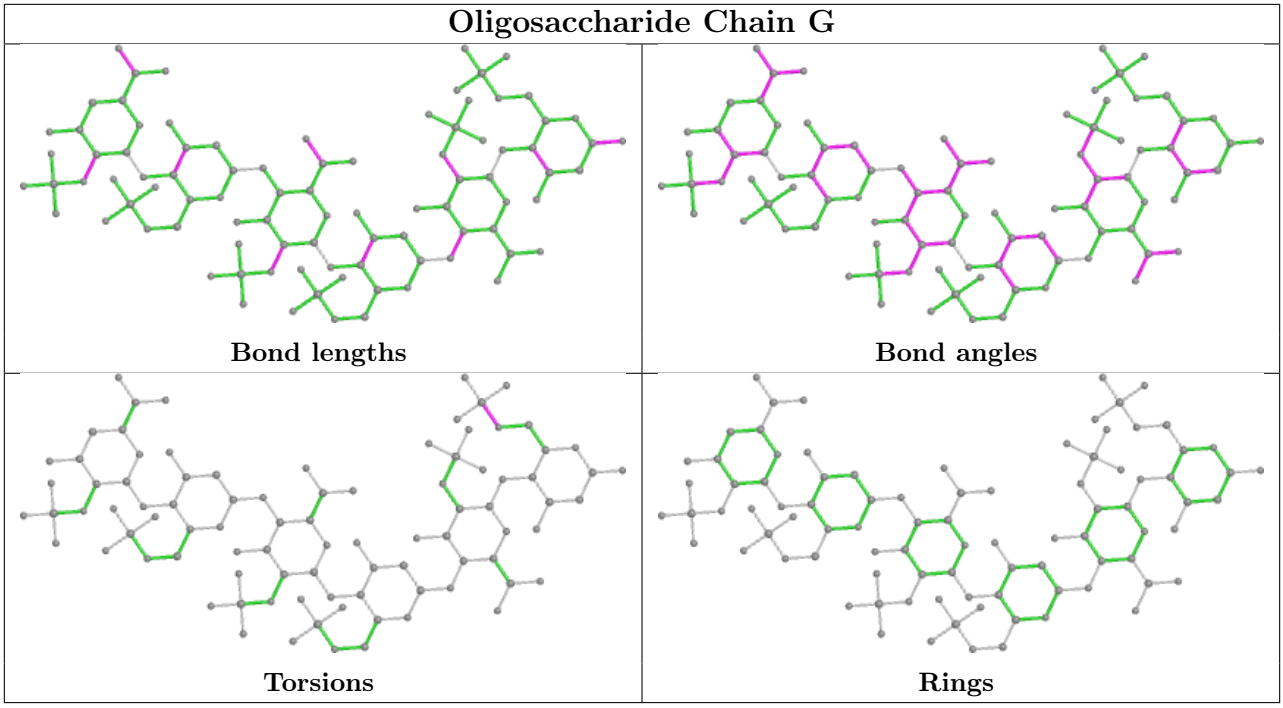


Rings



5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	427/427 (100%)	-0.27	12 (2%)	53	43	19, 38, 86, 131	0
1	B	427/427 (100%)	-0.15	13 (3%)	50	40	20, 36, 88, 133	0
1	C	427/427 (100%)	-0.10	10 (2%)	60	51	20, 39, 95, 144	0
1	D	425/427 (99%)	-0.09	16 (3%)	40	30	18, 39, 94, 141	0
1	E	425/427 (99%)	-0.19	11 (2%)	56	46	19, 34, 81, 115	0
All	All	2131/2135 (99%)	-0.16	62 (2%)	51	41	18, 37, 91, 144	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	434	GLY	4.9
1	B	403	ASN	4.6
1	D	434	GLY	4.6
1	E	403	ASN	4.5
1	E	435	SER	4.5
1	B	136	ALA	4.5
1	B	56	ASN	4.4
1	E	434	GLY	4.3
1	A	138	ASN	4.1
1	A	55	PRO	3.7
1	E	141	VAL	3.7
1	B	435	SER	3.6
1	B	436	GLY	3.5
1	B	178	VAL	3.5
1	B	176	THR	3.4
1	D	443	LYS	3.4
1	C	435	SER	3.3
1	C	436	GLY	3.2
1	A	139	ALA	3.2
1	D	435	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	283	THR	3.0
1	D	403	ASN	2.9
1	C	438	GLU	2.9
1	D	90	PHE	2.9
1	C	433	GLY	2.9
1	E	436	GLY	2.8
1	B	434	GLY	2.7
1	A	435	SER	2.6
1	D	396	SER	2.6
1	C	139	ALA	2.6
1	E	353	THR	2.6
1	C	474	LEU	2.6
1	B	137	ALA	2.5
1	D	432	GLY	2.5
1	D	141	VAL	2.5
1	B	141	VAL	2.5
1	C	434	GLY	2.5
1	A	61	LEU	2.4
1	E	140	GLY	2.4
1	B	474	LEU	2.3
1	E	433	GLY	2.3
1	D	433	GLY	2.3
1	E	139	ALA	2.3
1	C	176	THR	2.2
1	D	353	THR	2.2
1	A	58	ASN	2.2
1	A	353	THR	2.2
1	D	40	SER	2.2
1	D	438	GLU	2.2
1	E	175	CYS	2.2
1	A	137	ALA	2.1
1	B	177	ASN	2.1
1	D	436	GLY	2.1
1	D	85	PHE	2.1
1	A	433	GLY	2.1
1	E	55	PRO	2.1
1	D	176	THR	2.1
1	C	142	ASP	2.1
1	B	315	ARG	2.1
1	A	56	ASN	2.1
1	C	56	ASN	2.0
1	A	437	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

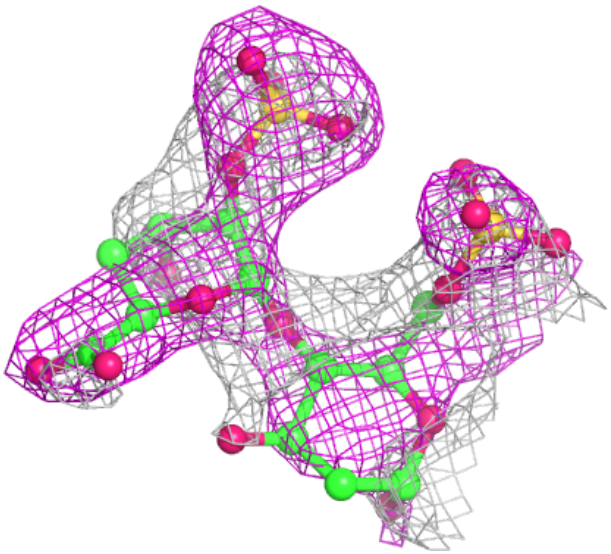
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

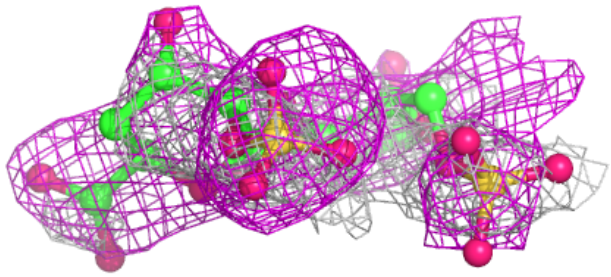
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	JHM	J	1	15/15	0.33	0.96	46,66,88,89	0
2	JHM	L	1	15/15	0.34	0.68	46,66,88,89	0
3	JHM	G	1	15/15	0.38	0.73	46,66,88,89	0
2	JHM	I	1	15/15	0.42	0.84	46,66,88,89	0
2	JHM	O	1	15/15	0.46	0.41	46,66,88,89	0
2	JHM	H	1	15/15	0.47	0.60	46,66,88,89	0
3	JHM	G	5	14/15	0.47	0.55	46,66,88,89	0
3	IDS	G	2	16/17	0.50	0.72	30,32,42,69	0
2	JHM	N	1	15/15	0.51	0.43	46,66,88,89	0
2	IDS	J	2	15/17	0.53	0.90	30,31,38,42	0
2	IDS	K	2	15/17	0.54	0.77	30,31,38,42	0
2	JHM	M	1	15/15	0.57	0.53	46,66,88,89	0
3	JHM	G	3	14/15	0.57	0.70	46,66,88,89	0
2	JHM	K	1	15/15	0.57	0.68	46,66,88,89	0
2	IDS	O	2	15/17	0.61	0.47	30,31,38,42	0
2	JHM	P	1	15/15	0.61	0.42	46,66,88,89	0
2	IDS	H	2	15/17	0.65	0.72	30,31,38,42	0
2	JHM	F	1	15/15	0.65	0.65	46,66,88,89	0
2	IDS	I	2	15/17	0.67	0.69	30,31,38,42	0
2	IDS	P	2	15/17	0.67	0.46	30,31,38,42	0
2	IDS	F	2	15/17	0.69	0.73	30,31,38,42	0
2	IDS	M	2	15/17	0.74	0.65	30,31,38,42	0
2	IDS	L	2	15/17	0.75	0.64	30,31,38,42	0
3	IDS	G	4	16/17	0.76	0.70	30,32,42,69	0
3	IDS	G	6	15/17	0.77	0.72	30,31,38,42	0
2	IDS	N	2	15/17	0.78	0.51	30,31,38,42	0

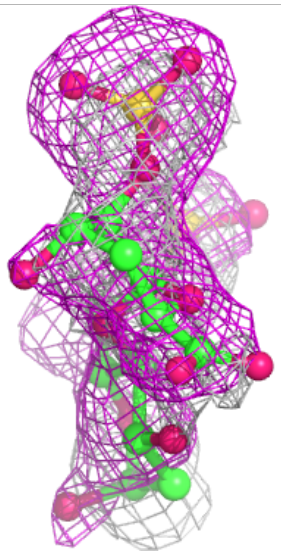
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain F:

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

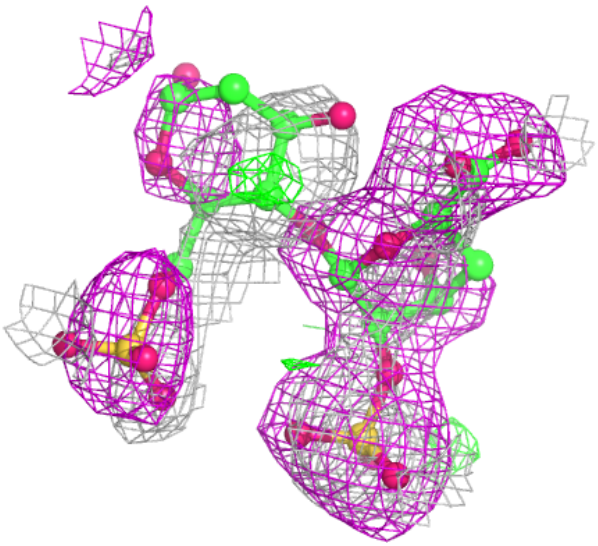


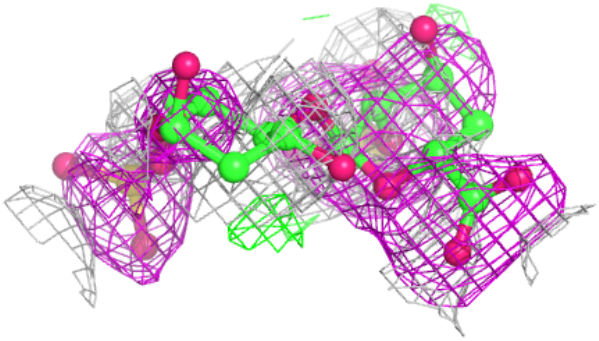


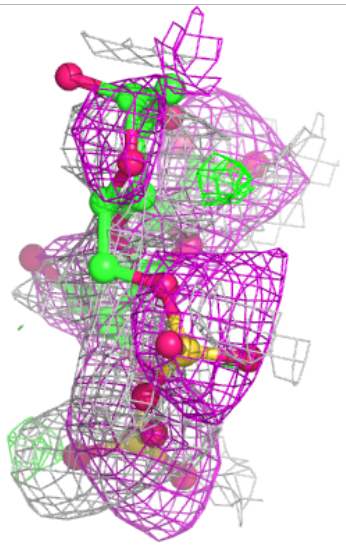


Electron density around Chain H:

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

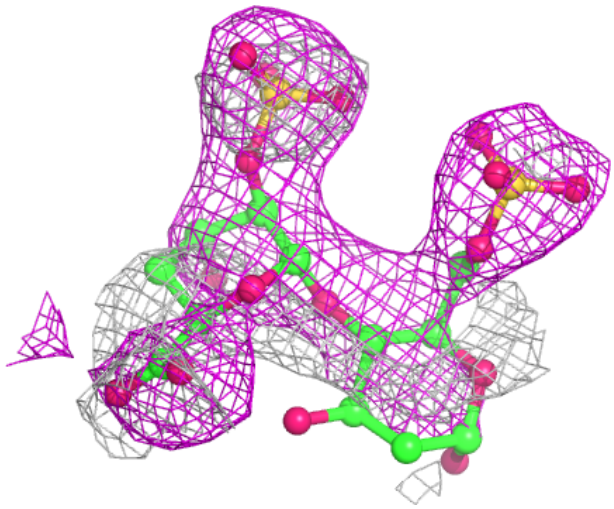


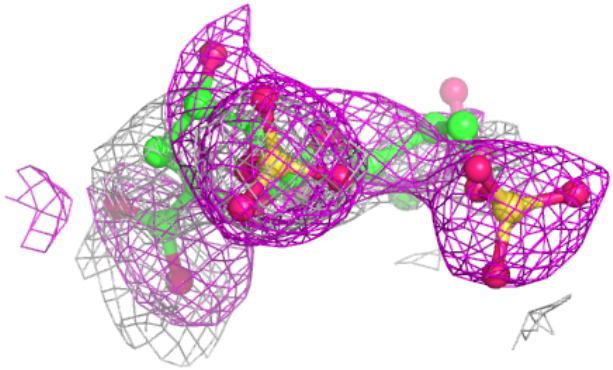


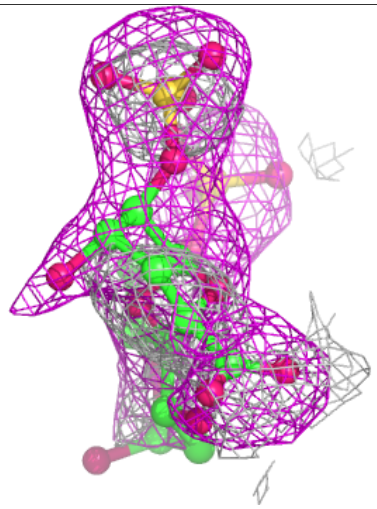


Electron density around Chain I:

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

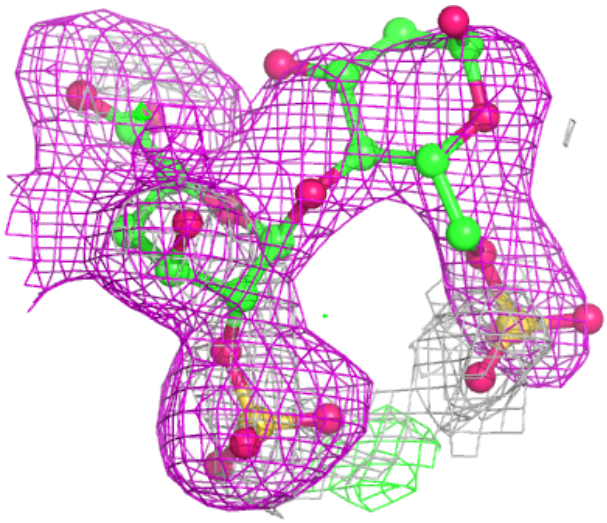


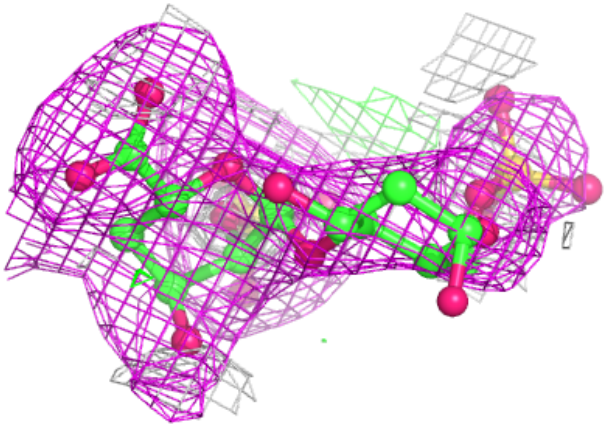


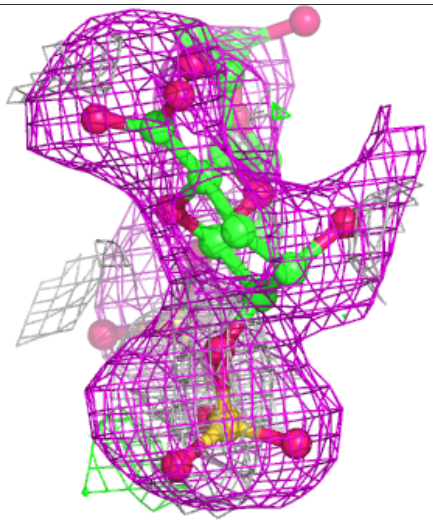


Electron density around Chain J:

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

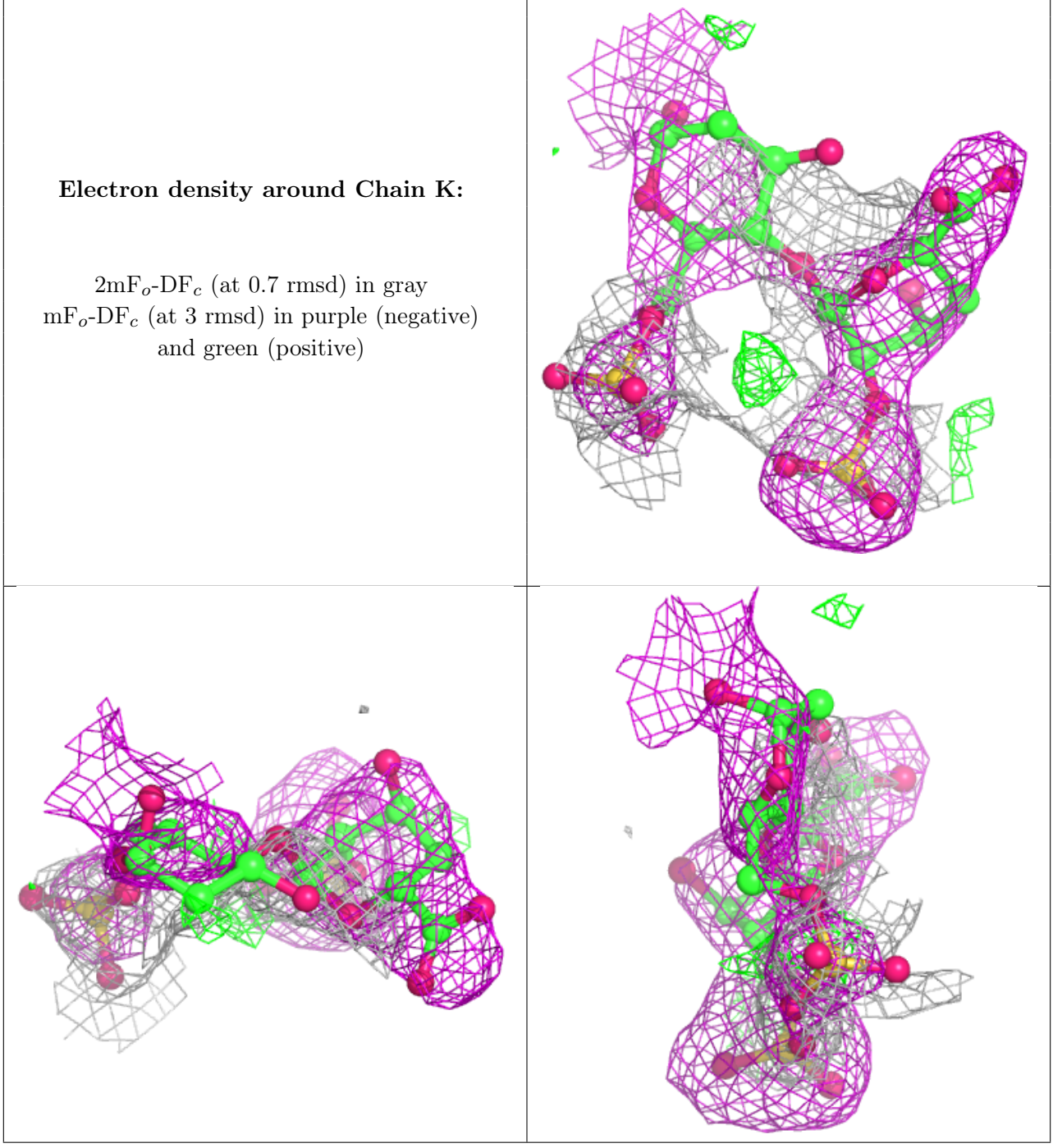






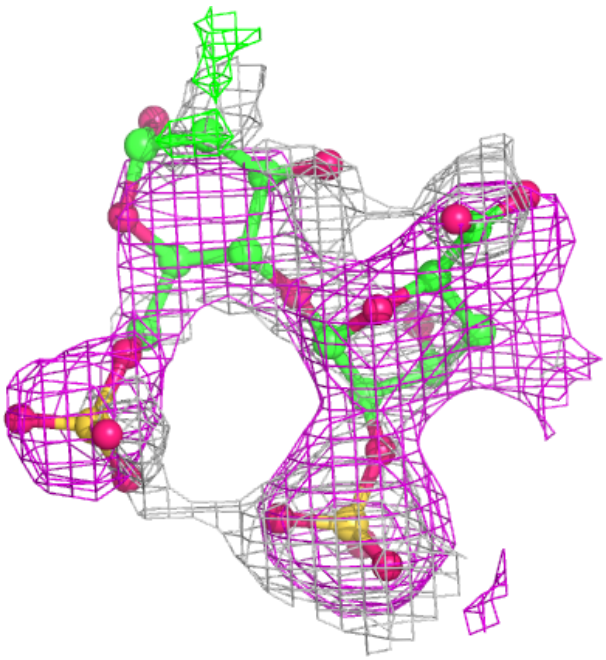
Electron density around Chain K:

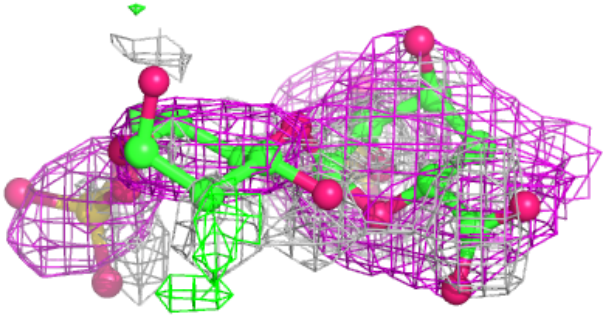
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

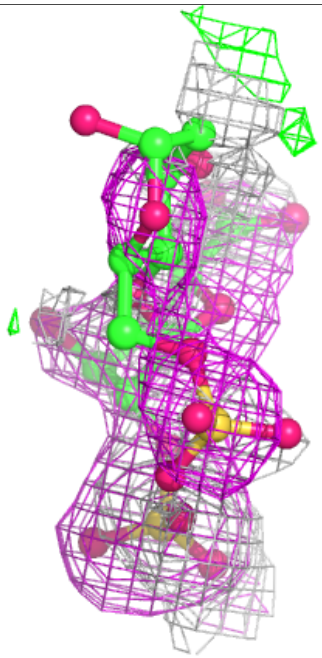


Electron density around Chain L:

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

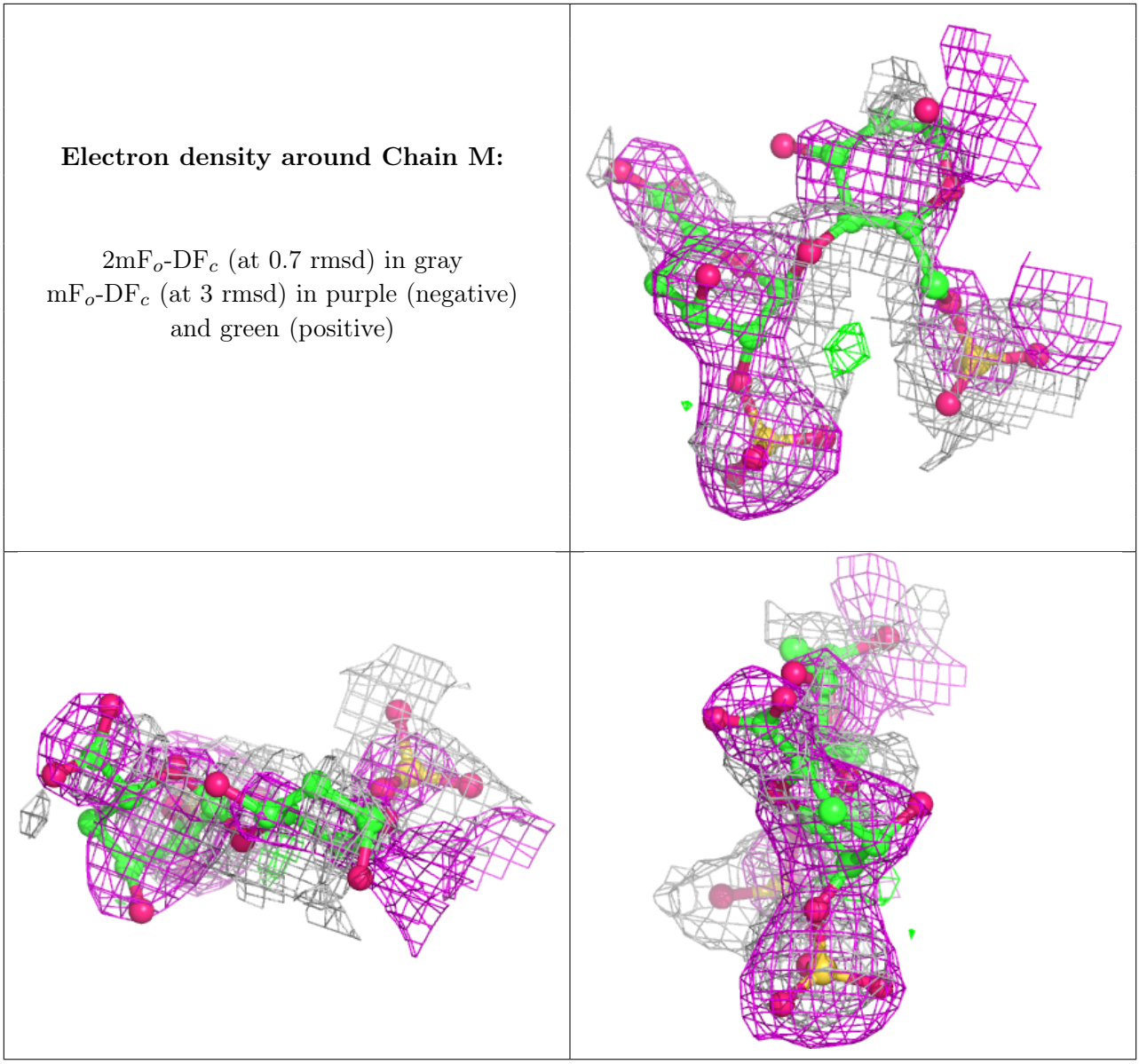






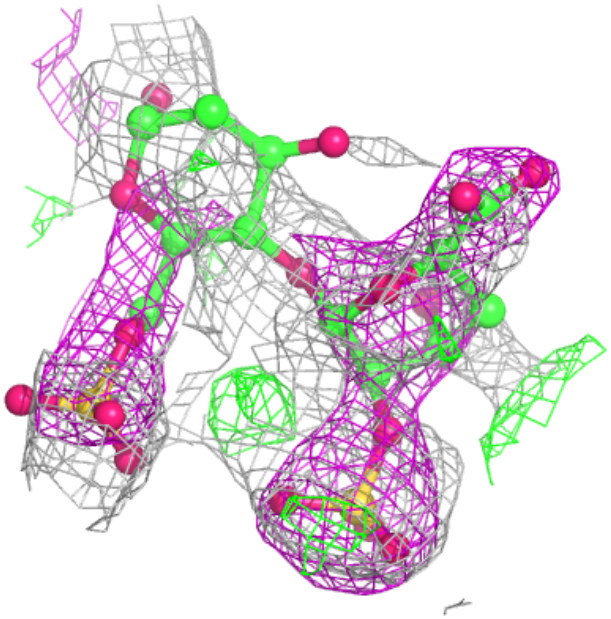
Electron density around Chain M:

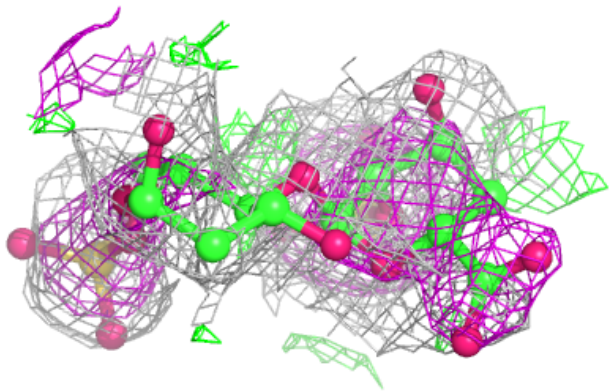
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

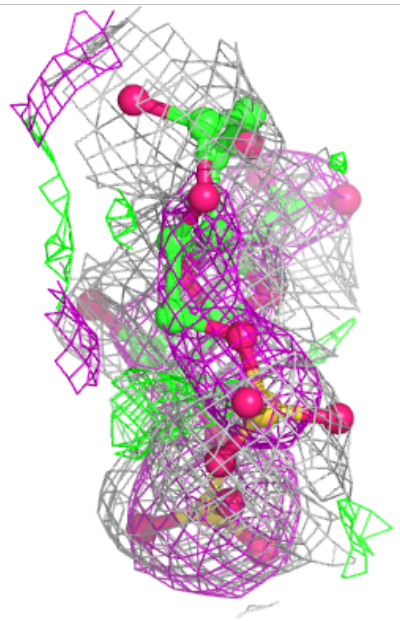


Electron density around Chain N:

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

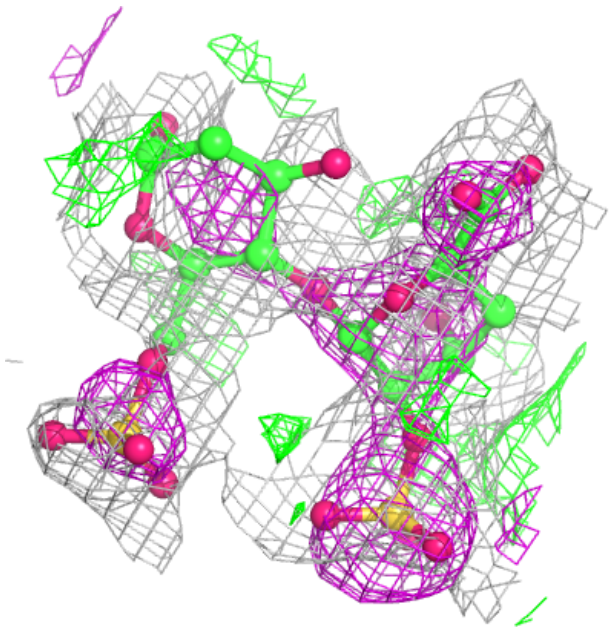


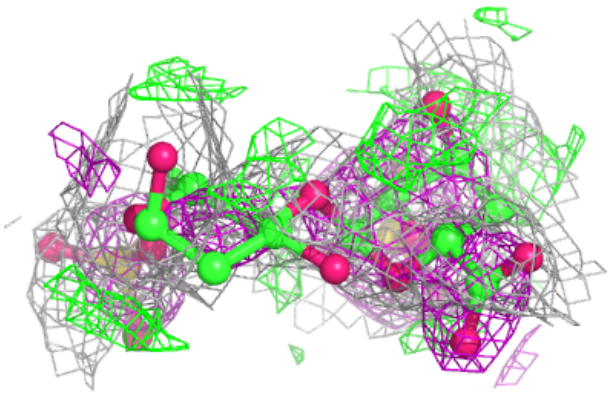


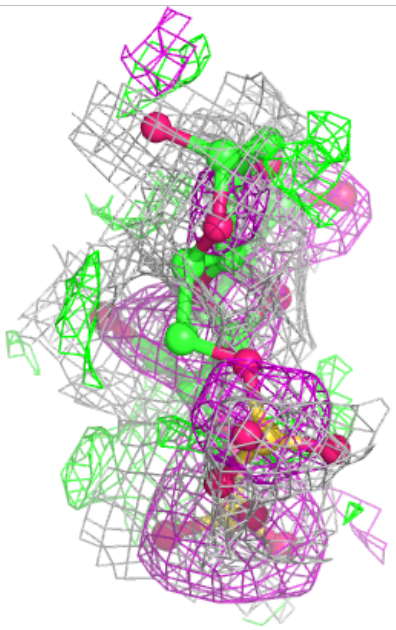


Electron density around Chain O:

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

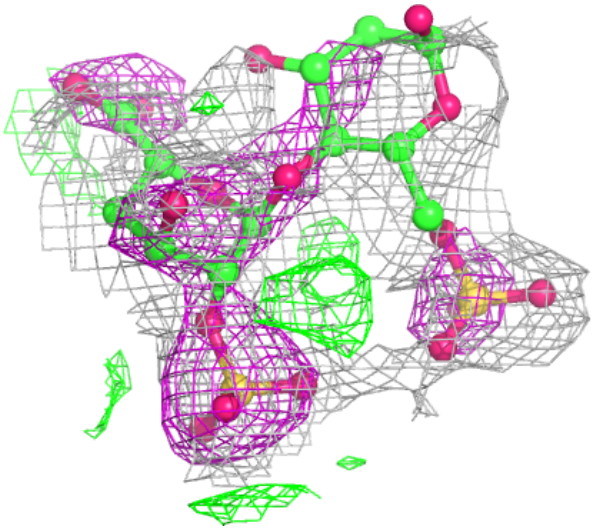


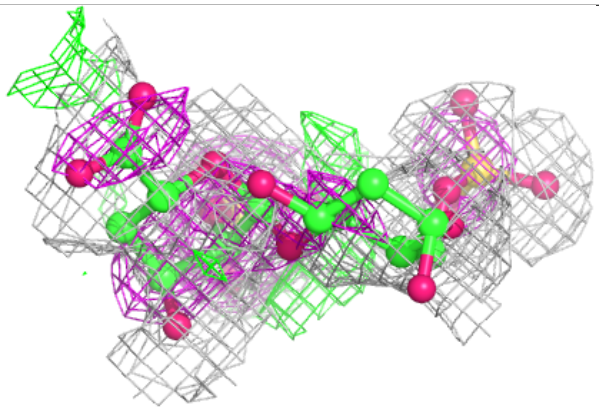


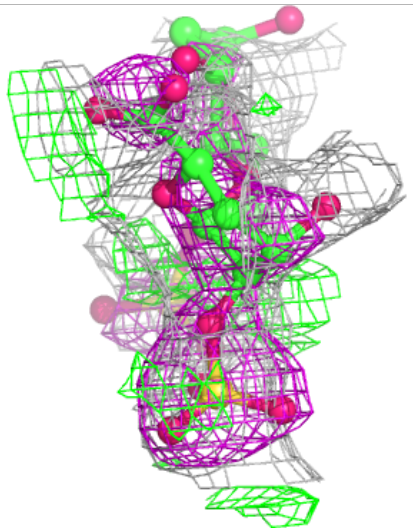


Electron density around Chain P:

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

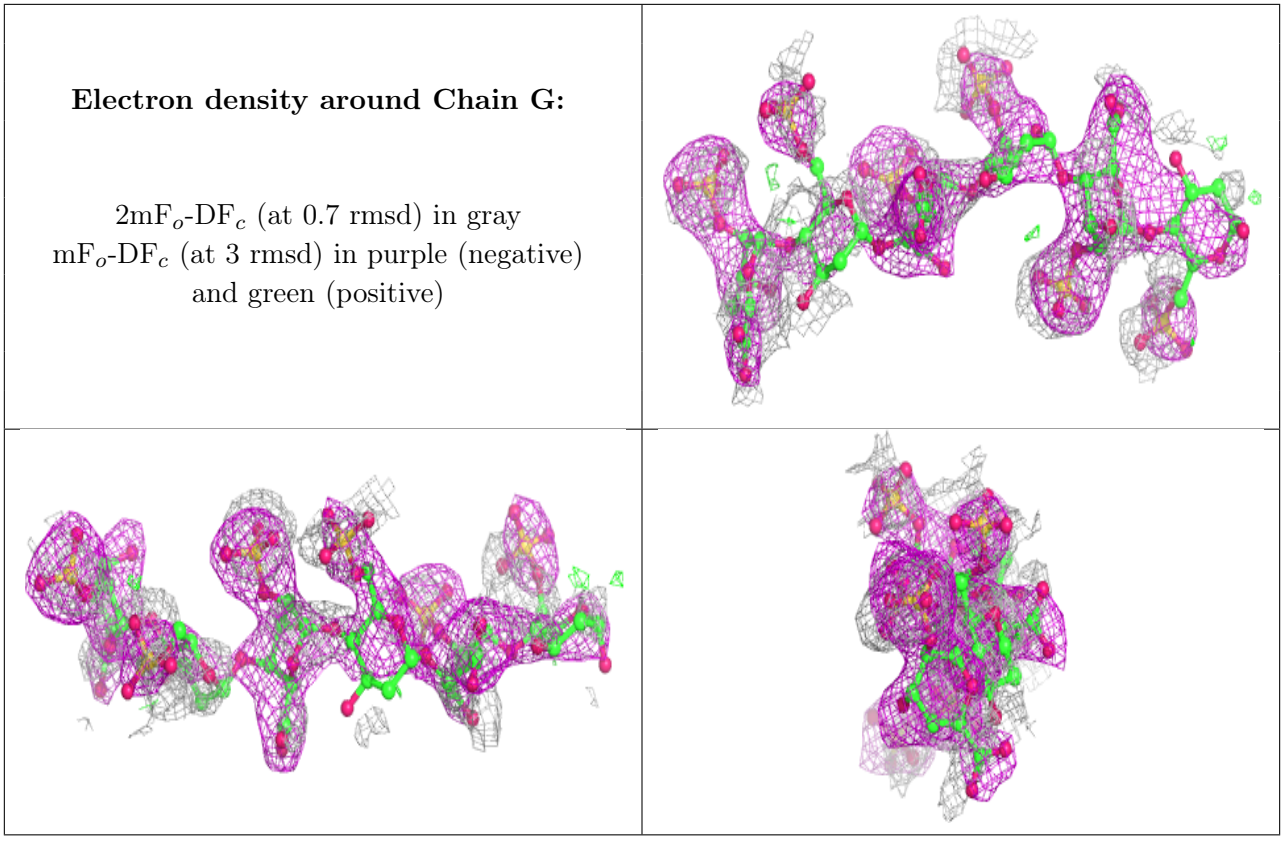






Electron density around Chain G:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.