



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 11:27 PM BST

PDB ID : 6LF3
Title : 3D domain-swapped dimer of the maltose-binding protein fused to a fragment of the protein-tyrosine kinase 2-beta
Authors : Momin, A.A.; Shahul Hameed, U.F.; Arold, S.T.
Deposited on : 2019-11-28
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

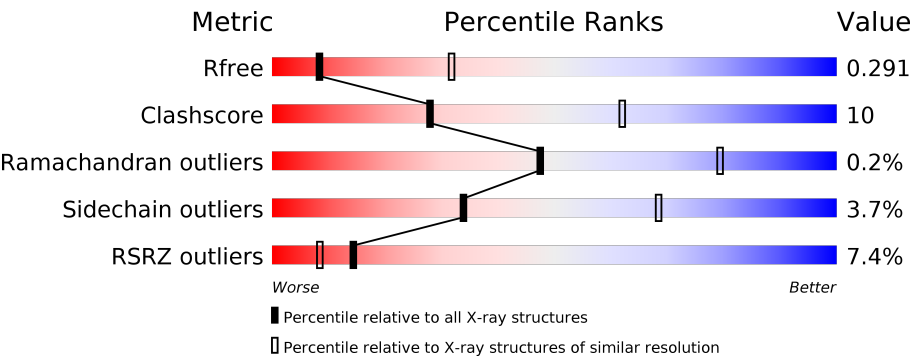
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	419	<div><div>3%</div><div></div><div>71%</div><div>16%</div><div>•</div><div>12%</div></div>
1	B	419	<div><div>4%</div><div></div><div>73%</div><div>14%</div><div>•</div><div>12%</div></div>
1	C	419	<div><div>9%</div><div></div><div>70%</div><div>17%</div><div>•</div><div>12%</div></div>
1	D	419	<div><div>10%</div><div></div><div>68%</div><div>17%</div><div>•</div><div>12%</div></div>
1	E	419	<div><div>7%</div><div></div><div>71%</div><div>16%</div><div></div><div>12%</div></div>
1	F	419	<div><div>6%</div><div></div><div>73%</div><div>14%</div><div>•</div><div>12%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	2	 50%50%
2	H	2	 50%50%
2	I	2	 100%
2	J	2	 50%50%
2	K	2	 50%50%
2	L	2	 50%50%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17124 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 Maltose/maltodextrin-binding periplasmic protein,Protein-tyrosine kinase 2-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2837	1827	463	541	6			
1	B	369	Total	C	N	O	S	0	0	0
			2837	1827	463	541	6			
1	C	368	Total	C	N	O	S	0	0	0
			2828	1822	462	538	6			
1	D	368	Total	C	N	O	S	0	0	0
			2828	1822	462	538	6			
1	E	368	Total	C	N	O	S	0	0	0
			2828	1822	462	538	6			
1	F	368	Total	C	N	O	S	0	0	0
			2828	1822	462	538	6			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0AEX9
A	83	ALA	ASP	engineered mutation	UNP P0AEX9
A	84	ALA	LYS	engineered mutation	UNP P0AEX9
A	173	ALA	GLU	engineered mutation	UNP P0AEX9
A	174	ALA	ASN	engineered mutation	UNP P0AEX9
A	240	ALA	LYS	engineered mutation	UNP P0AEX9
A	360	ALA	GLU	engineered mutation	UNP P0AEX9
A	363	ALA	LYS	engineered mutation	UNP P0AEX9
A	364	ALA	ASP	engineered mutation	UNP P0AEX9
A	368	ASN	-	linker	UNP P0AEX9
A	369	ALA	-	linker	UNP P0AEX9
B	1	MET	-	initiating methionine	UNP P0AEX9
B	83	ALA	ASP	engineered mutation	UNP P0AEX9
B	84	ALA	LYS	engineered mutation	UNP P0AEX9
B	173	ALA	GLU	engineered mutation	UNP P0AEX9
B	174	ALA	ASN	engineered mutation	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	240	ALA	LYS	engineered mutation	UNP P0AEX9
B	360	ALA	GLU	engineered mutation	UNP P0AEX9
B	363	ALA	LYS	engineered mutation	UNP P0AEX9
B	364	ALA	ASP	engineered mutation	UNP P0AEX9
B	368	ASN	-	linker	UNP P0AEX9
B	369	ALA	-	linker	UNP P0AEX9
C	1	MET	-	initiating methionine	UNP P0AEX9
C	83	ALA	ASP	engineered mutation	UNP P0AEX9
C	84	ALA	LYS	engineered mutation	UNP P0AEX9
C	173	ALA	GLU	engineered mutation	UNP P0AEX9
C	174	ALA	ASN	engineered mutation	UNP P0AEX9
C	240	ALA	LYS	engineered mutation	UNP P0AEX9
C	360	ALA	GLU	engineered mutation	UNP P0AEX9
C	363	ALA	LYS	engineered mutation	UNP P0AEX9
C	364	ALA	ASP	engineered mutation	UNP P0AEX9
C	368	ASN	-	linker	UNP P0AEX9
C	369	ALA	-	linker	UNP P0AEX9
D	1	MET	-	initiating methionine	UNP P0AEX9
D	83	ALA	ASP	engineered mutation	UNP P0AEX9
D	84	ALA	LYS	engineered mutation	UNP P0AEX9
D	173	ALA	GLU	engineered mutation	UNP P0AEX9
D	174	ALA	ASN	engineered mutation	UNP P0AEX9
D	240	ALA	LYS	engineered mutation	UNP P0AEX9
D	360	ALA	GLU	engineered mutation	UNP P0AEX9
D	363	ALA	LYS	engineered mutation	UNP P0AEX9
D	364	ALA	ASP	engineered mutation	UNP P0AEX9
D	368	ASN	-	linker	UNP P0AEX9
D	369	ALA	-	linker	UNP P0AEX9
E	1	MET	-	initiating methionine	UNP P0AEX9
E	83	ALA	ASP	engineered mutation	UNP P0AEX9
E	84	ALA	LYS	engineered mutation	UNP P0AEX9
E	173	ALA	GLU	engineered mutation	UNP P0AEX9
E	174	ALA	ASN	engineered mutation	UNP P0AEX9
E	240	ALA	LYS	engineered mutation	UNP P0AEX9
E	360	ALA	GLU	engineered mutation	UNP P0AEX9
E	363	ALA	LYS	engineered mutation	UNP P0AEX9
E	364	ALA	ASP	engineered mutation	UNP P0AEX9
E	368	ASN	-	linker	UNP P0AEX9
E	369	ALA	-	linker	UNP P0AEX9
F	1	MET	-	initiating methionine	UNP P0AEX9
F	83	ALA	ASP	engineered mutation	UNP P0AEX9
F	84	ALA	LYS	engineered mutation	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	173	ALA	GLU	engineered mutation	UNP P0AEX9
F	174	ALA	ASN	engineered mutation	UNP P0AEX9
F	240	ALA	LYS	engineered mutation	UNP P0AEX9
F	360	ALA	GLU	engineered mutation	UNP P0AEX9
F	363	ALA	LYS	engineered mutation	UNP P0AEX9
F	364	ALA	ASP	engineered mutation	UNP P0AEX9
F	368	ASN	-	linker	UNP P0AEX9
F	369	ALA	-	linker	UNP P0AEX9

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

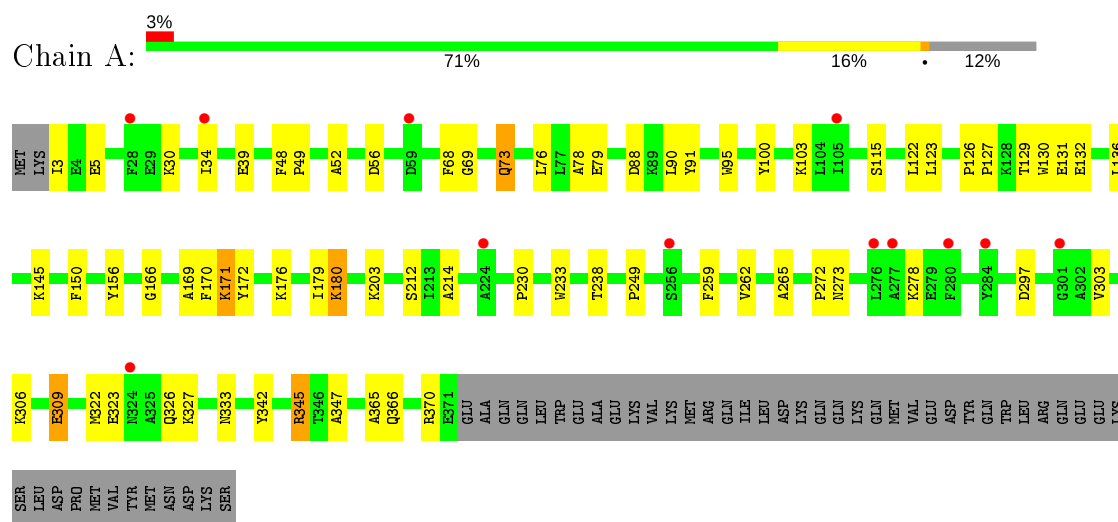


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			
2	I	2	Total	C	O	0	0	0
			23	12	11			
2	J	2	Total	C	O	0	0	0
			23	12	11			
2	K	2	Total	C	O	0	0	0
			23	12	11			
2	L	2	Total	C	O	0	0	0
			23	12	11			

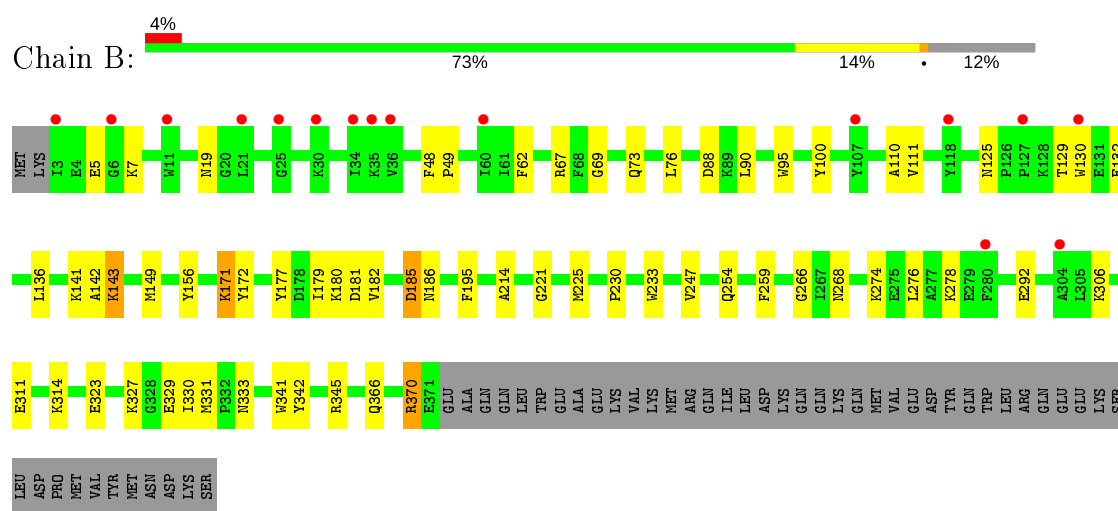
3 Residue-property plots [i](#)

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.

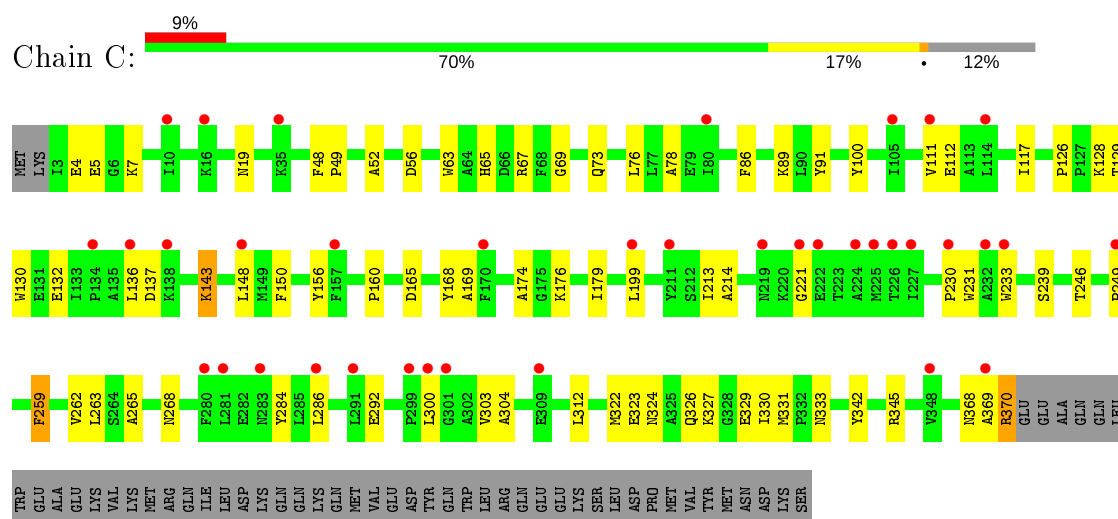
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein,Protein-tyrosine kinase 2-beta



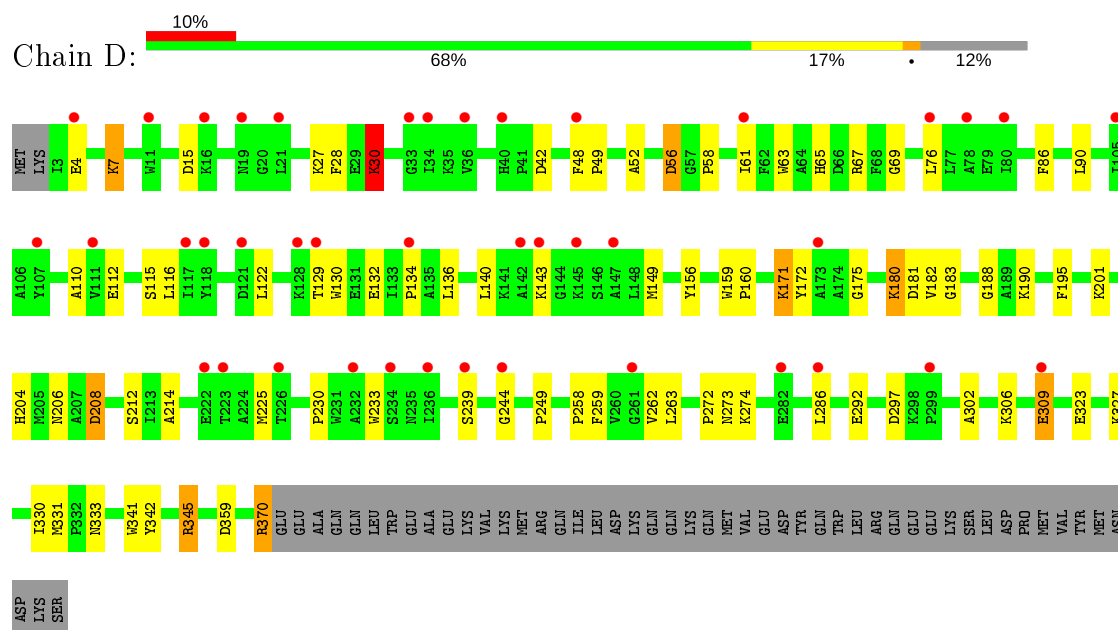
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein,Protein-tyrosine kinase 2-beta



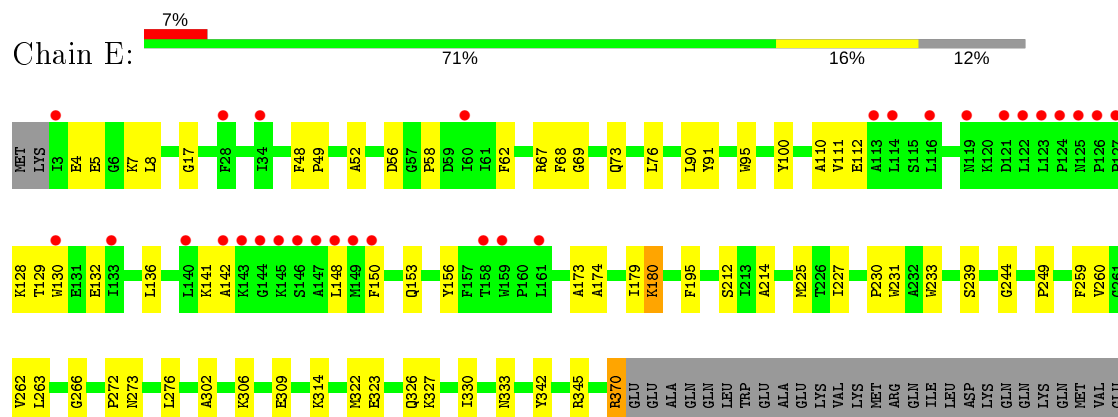
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein,Protein-tyrosine kinase 2-beta



- Molecule 1: Maltose/maltodextrin-binding periplasmic protein,Protein-tyrosine kinase 2-beta



- Molecule 1: Maltose/maltodextrin-binding periplasmic protein,Protein-tyrosine kinase 2-beta





- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.78Å 92.74Å 93.61Å 112.46° 101.66° 94.93°	Depositor
Resolution (Å)	47.90 – 3.20 47.86 – 3.21	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.90-3.20) 97.0 (47.86-3.21)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.244 , 0.284 0.250 , 0.291	Depositor DCC
R_{free} test set	1864 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	99.1	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 87.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17124	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GLC

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	0.41	0/2906	0.74	2/3951 (0.1%)
1	B	0.41	0/2906	0.71	0/3951
1	C	0.36	0/2897	0.68	0/3939
1	D	0.39	0/2897	0.74	4/3939 (0.1%)
1	E	0.39	0/2897	0.69	0/3939
1	F	0.40	0/2897	0.71	0/3939
All	All	0.40	0/17400	0.71	6/23658 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	F	0	2
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	201	LYS	CB-CG-CD	6.49	128.47	111.60
1	D	30	LYS	CB-CA-C	6.07	122.54	110.40
1	A	345	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	D	56	ASP	CB-CA-C	5.36	121.12	110.40
1	D	345	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	309	GLU	CB-CG-CD	5.11	127.99	114.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	173	ALA	Peptide
1	F	173	ALA	Peptide
1	F	174	ALA	Peptide

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	2837	0	2804	84	0
1	B	2837	0	2804	70	1
1	C	2828	0	2798	80	0
1	D	2828	0	2798	89	0
1	E	2828	0	2798	77	1
1	F	2828	0	2798	63	0
2	G	23	0	21	3	0
2	H	23	0	21	4	0
2	I	23	0	21	7	0
2	J	23	0	21	5	0
2	K	23	0	21	4	0
2	L	23	0	21	3	0
All	All	17124	0	16926	337	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 10.

All (337) 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:A:366:GLN:HE21	1:A:370:ARG:NH2	1.38	1.20
1:D:180:LYS:HE2	1:D:180:LYS:HA	1.20	1.15
1:B:185:ASP:OD1	1:B:366:GLN:OE1	1.64	1.15
1:A:203:LYS:CG	1:E:314:LYS:HB3	1.77	1.12
1:F:156:TYR:HB2	2:L:1:GLC:H62	1.19	1.11
1:B:156:TYR:HB2	2:H:1:GLC:H62	1.28	1.10
1:B:142:ALA:HB1	1:E:323:GLU:OE1	1.50	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LYS:HG3	1:E:314:LYS:CB	1.83	1.06
1:A:366:GLN:NE2	1:A:370:ARG:NH2	2.04	1.06
1:A:180:LYS:HE2	1:A:370:ARG:HD3	1.33	1.06
1:F:370:ARG:HG2	1:F:370:ARG:HH11	1.23	1.01
1:B:185:ASP:OD2	1:B:366:GLN:HG2	1.60	1.00
1:E:156:TYR:HB2	2:K:1:GLC:H62	1.41	0.99
1:A:156:TYR:HB2	2:G:1:GLC:H62	1.46	0.94
1:D:156:TYR:HB2	2:J:1:GLC:H61	1.48	0.94
1:A:366:GLN:NE2	1:A:370:ARG:HH21	1.64	0.93
1:D:180:LYS:CE	1:D:180:LYS:HA	1.97	0.93
1:A:90:LEU:HD13	1:A:95:TRP:CZ2	2.05	0.92
1:D:156:TYR:HB2	2:J:1:GLC:C6	2.00	0.92
1:C:263:LEU:HB2	1:D:112:GLU:OE2	1.69	0.92
1:B:90:LEU:HD13	1:B:95:TRP:CZ2	2.05	0.92
1:C:174:ALA:O	1:D:175:GLY:HA2	1.68	0.91
1:E:180:LYS:HE2	1:E:370:ARG:HG2	1.52	0.90
1:E:273:ASN:OD1	1:F:5:GLU:HG2	1.72	0.90
1:D:67:ARG:NH1	2:J:1:GLC:O2	2.04	0.90
1:F:156:TYR:HB2	2:L:1:GLC:C6	2.03	0.88
1:B:142:ALA:CB	1:E:323:GLU:OE1	2.23	0.87
1:F:156:TYR:CB	2:L:1:GLC:H62	2.04	0.86
1:A:203:LYS:HG3	1:E:314:LYS:HB3	0.89	0.86
1:A:73:GLN:HG3	1:A:100:TYR:OH	1.74	0.86
1:B:185:ASP:OD2	1:B:366:GLN:CG	2.24	0.84
1:E:156:TYR:HB2	2:K:1:GLC:C6	2.08	0.83
1:D:7:LYS:NZ	1:D:7:LYS:HB2	1.92	0.83
1:A:129:THR:HG23	1:A:132:GLU:HG2	1.61	0.82
1:D:63:TRP:HE1	2:J:1:GLC:HO3	1.23	0.82
1:A:180:LYS:HE2	1:A:370:ARG:CD	2.10	0.81
1:A:366:GLN:HE21	1:A:370:ARG:HH22	1.24	0.81
1:A:172:TYR:HB2	1:B:177:TYR:CE1	2.15	0.80
1:C:69:GLY:HA3	1:D:333:ASN:O	1.82	0.80
1:B:156:TYR:HB2	2:H:1:GLC:C6	2.11	0.80
1:E:333:ASN:O	1:F:69:GLY:HA3	1.83	0.79
1:A:366:GLN:HE21	1:A:370:ARG:HH21	1.17	0.79
1:C:130:TRP:HB3	1:D:195:PHE:HE2	1.45	0.79
1:E:272:PRO:HB2	1:F:5:GLU:HG3	1.64	0.78
1:B:156:TYR:CB	2:H:1:GLC:H62	2.11	0.77
1:E:156:TYR:CB	2:K:1:GLC:H62	2.15	0.76
1:E:4:GLU:HB2	1:E:7:LYS:HD2	1.67	0.76
1:B:370:ARG:O	1:B:370:ARG:HG2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:GLU:HB2	1:E:7:LYS:CD	2.17	0.74
1:A:69:GLY:HA3	1:B:333:ASN:O	1.88	0.74
1:C:4:GLU:HB3	1:C:7:LYS:CD	2.17	0.74
1:C:86:PHE:HZ	1:D:286:LEU:CD1	2.01	0.73
1:E:4:GLU:CB	1:E:7:LYS:HD2	2.18	0.73
1:C:4:GLU:HB3	1:C:7:LYS:HD2	1.71	0.72
1:A:145:LYS:HE3	1:B:221:GLY:O	1.88	0.72
1:C:86:PHE:HZ	1:D:286:LEU:HD13	1.54	0.71
1:B:67:ARG:HD3	2:H:1:GLC:O2	1.88	0.71
1:A:129:THR:CG2	1:A:132:GLU:HG2	2.20	0.71
1:A:78:ALA:HB2	1:B:274:LYS:HE3	1.73	0.71
1:F:171:LYS:HE3	1:F:172:TYR:H	1.54	0.71
1:C:112:GLU:OE2	1:D:263:LEU:HB2	1.89	0.71
1:B:171:LYS:HE3	1:B:172:TYR:H	1.55	0.70
1:B:180:LYS:HE2	1:B:370:ARG:HG3	1.72	0.70
1:E:90:LEU:HD12	1:E:95:TRP:CZ2	2.27	0.70
1:E:5:GLU:HG2	1:F:272:PRO:HB2	1.74	0.70
1:B:185:ASP:OD1	1:B:366:GLN:CD	2.30	0.69
1:A:171:LYS:HB2	1:B:181:ASP:OD2	1.92	0.69
1:D:4:GLU:HB3	1:D:7:LYS:CD	2.24	0.68
1:A:169:ALA:O	1:B:182:VAL:HA	1.93	0.68
1:A:156:TYR:CB	2:G:1:GLC:H62	2.23	0.68
1:F:370:ARG:HG2	1:F:370:ARG:NH1	1.99	0.67
1:E:129:THR:OG1	1:E:132:GLU:HG3	1.95	0.67
1:A:333:ASN:O	1:B:69:GLY:HA3	1.94	0.67
1:C:129:THR:OG1	1:C:132:GLU:HG3	1.95	0.67
1:E:69:GLY:HA3	1:F:333:ASN:O	1.96	0.66
1:A:171:LYS:HD3	1:A:172:TYR:H	1.61	0.65
1:C:331:MET:O	1:D:65:HIS:NE2	2.27	0.65
1:A:272:PRO:HB2	1:B:5:GLU:HG3	1.78	0.65
1:D:129:THR:OG1	1:D:132:GLU:HG3	1.96	0.65
1:E:244:GLY:HA3	1:F:120:LYS:HE2	1.78	0.65
1:F:129:THR:OG1	1:F:132:GLU:HG3	1.96	0.65
1:B:129:THR:OG1	1:B:132:GLU:HG3	1.96	0.65
1:D:4:GLU:HB3	1:D:7:LYS:HD2	1.77	0.64
1:B:90:LEU:HD13	1:B:95:TRP:HZ2	1.58	0.64
1:A:129:THR:OG1	1:A:131:GLU:OE1	2.16	0.64
1:C:156:TYR:HB2	2:I:1:GLC:H62	1.80	0.64
1:C:213:ILE:HG22	1:D:149:MET:CE	2.28	0.63
1:D:342:TYR:HD1	1:D:345:ARG:HH12	1.47	0.63
1:E:195:PHE:HE2	1:F:130:TRP:HB3	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ASN:O	1:D:69:GLY:HA3	1.98	0.63
1:A:342:TYR:HD1	1:A:345:ARG:NH1	1.96	0.63
1:C:86:PHE:CZ	1:D:286:LEU:HD13	2.34	0.63
1:A:170:PHE:HA	1:B:181:ASP:O	1.99	0.63
1:C:130:TRP:HB3	1:D:195:PHE:CE2	2.32	0.63
1:C:213:ILE:HG22	1:D:149:MET:HE1	1.81	0.63
1:A:322:MET:O	1:A:326:GLN:HG3	1.99	0.62
1:A:370:ARG:HG3	1:A:370:ARG:O	1.99	0.62
1:C:156:TYR:HB2	2:I:1:GLC:C6	2.29	0.62
1:D:7:LYS:HB2	1:D:7:LYS:HZ1	1.63	0.62
1:D:342:TYR:HD1	1:D:345:ARG:NH1	1.98	0.61
1:C:370:ARG:C	1:C:370:ARG:HH11	2.03	0.61
1:A:156:TYR:HB2	2:G:1:GLC:C6	2.27	0.61
1:C:168:TYR:OH	1:D:181:ASP:OD1	2.18	0.61
1:E:91:TYR:CZ	1:F:306:LYS:HG2	2.35	0.61
1:A:88:ASP:O	1:B:306:LYS:NZ	2.18	0.61
1:C:322:MET:O	1:C:326:GLN:HG3	2.01	0.61
1:D:7:LYS:NZ	1:D:7:LYS:CB	2.65	0.60
1:A:366:GLN:CD	1:A:370:ARG:HH21	2.04	0.60
1:B:180:LYS:HD3	1:B:180:LYS:O	2.02	0.60
1:F:150:PHE:CE1	1:F:152:LEU:HD21	2.37	0.59
1:A:366:GLN:CG	1:A:370:ARG:HH21	2.16	0.59
1:C:5:GLU:HG3	1:D:272:PRO:HB2	1.84	0.59
1:F:322:MET:O	1:F:326:GLN:HG3	2.02	0.59
1:E:370:ARG:C	1:E:370:ARG:HD2	2.22	0.59
1:C:78:ALA:HB2	1:D:274:LYS:HE3	1.85	0.58
1:B:247:VAL:HG22	1:B:323:GLU:CD	2.24	0.58
1:C:214:ALA:HA	1:D:149:MET:HE2	1.84	0.58
1:B:185:ASP:OD2	1:B:366:GLN:CB	2.52	0.58
1:E:244:GLY:CA	1:F:120:LYS:HE2	2.34	0.58
1:B:247:VAL:HG22	1:B:323:GLU:OE1	2.04	0.57
1:A:78:ALA:CB	1:B:274:LYS:HE3	2.34	0.57
1:A:90:LEU:HD13	1:A:95:TRP:HZ2	1.63	0.57
1:B:73:GLN:OE1	1:B:100:TYR:OH	2.12	0.57
1:E:342:TYR:HD1	1:E:345:ARG:NH1	2.02	0.57
1:E:73:GLN:OE1	1:E:100:TYR:OH	2.13	0.57
1:E:67:ARG:HD3	2:K:1:GLC:O2	2.04	0.57
1:E:322:MET:O	1:E:326:GLN:HG3	2.03	0.57
1:B:143:LYS:NZ	1:B:143:LYS:HB3	2.20	0.56
1:C:300:LEU:HB3	1:D:110:ALA:CB	2.36	0.55
1:E:17:GLY:HA3	1:F:297:ASP:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:PRO:HA	1:F:76:LEU:HD13	1.87	0.55
1:C:63:TRP:CH2	2:I:2:GLC:H61	2.41	0.55
1:C:67:ARG:NH1	2:I:1:GLC:O2	2.40	0.55
1:F:342:TYR:HD1	1:F:345:ARG:NH1	2.03	0.55
1:A:171:LYS:CB	1:B:181:ASP:OD2	2.54	0.54
1:E:141:LYS:NZ	1:F:203:LYS:O	2.37	0.54
1:C:174:ALA:O	1:D:175:GLY:CA	2.49	0.54
1:E:342:TYR:HD1	1:E:345:ARG:HH12	1.54	0.54
1:E:112:GLU:OE2	1:F:263:LEU:HB2	2.08	0.54
1:A:49:PRO:HA	1:A:76:LEU:HD13	1.89	0.54
1:D:156:TYR:HB2	2:J:1:GLC:H62	1.85	0.53
1:D:27:LYS:HA	1:D:30:LYS:HE2	1.89	0.53
1:B:185:ASP:CG	1:B:366:GLN:HB2	2.29	0.53
1:C:111:VAL:HG22	1:D:262:VAL:HG22	1.90	0.53
1:E:153:GLN:CG	1:F:210:ASP:HB3	2.39	0.53
1:C:265:ALA:HA	1:D:61:ILE:O	2.09	0.53
1:C:342:TYR:HD1	1:C:345:ARG:NH1	2.07	0.53
1:F:4:GLU:HB3	1:F:7:LYS:CD	2.39	0.53
1:C:370:ARG:HD3	1:C:370:ARG:C	2.30	0.52
1:B:311:GLU:HA	1:B:314:LYS:HE3	1.92	0.52
1:F:171:LYS:HE3	1:F:172:TYR:N	2.24	0.52
1:A:171:LYS:HD3	1:A:172:TYR:N	2.23	0.52
1:B:49:PRO:HA	1:B:76:LEU:HD13	1.89	0.52
1:E:111:VAL:HG22	1:F:262:VAL:HG22	1.92	0.52
1:A:265:ALA:HB2	1:B:62:PHE:CE1	2.45	0.52
1:D:206:ASN:OD1	1:D:208:ASP:HB2	2.09	0.52
1:E:260:VAL:CG1	1:F:111:VAL:HG13	2.40	0.51
1:E:276:LEU:HD22	1:F:34:ILE:HG13	1.92	0.51
1:E:130:TRP:NE1	1:F:249:PRO:HG2	2.25	0.51
1:E:4:GLU:CB	1:E:7:LYS:CD	2.84	0.51
1:C:73:GLN:OE1	1:C:100:TYR:OH	2.13	0.51
1:A:127:PRO:HD2	1:B:225:MET:SD	2.50	0.51
1:A:48:PHE:N	1:A:49:PRO:HD2	2.26	0.51
1:C:199:LEU:CD2	1:D:134:PRO:HG3	2.41	0.51
1:E:49:PRO:HA	1:E:76:LEU:HD13	1.92	0.51
1:E:153:GLN:HG3	1:F:210:ASP:HB3	1.92	0.51
1:E:273:ASN:OD1	1:F:5:GLU:HA	2.11	0.51
1:B:48:PHE:N	1:B:49:PRO:HD2	2.26	0.50
1:D:48:PHE:N	1:D:49:PRO:HD2	2.26	0.50
1:A:306:LYS:NZ	1:B:88:ASP:O	2.25	0.50
1:A:172:TYR:HB2	1:B:177:TYR:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:TRP:HB2	1:D:15:ASP:O	2.12	0.50
1:F:48:PHE:N	1:F:49:PRO:HD2	2.26	0.50
1:E:48:PHE:N	1:E:49:PRO:HD2	2.26	0.50
1:E:62:PHE:HZ	1:F:285:LEU:CD2	2.24	0.50
1:B:342:TYR:HD1	1:B:345:ARG:NH1	2.09	0.50
1:C:137:ASP:OD2	1:D:204:HIS:ND1	2.33	0.50
1:E:180:LYS:CE	1:E:370:ARG:HG2	2.32	0.50
1:C:48:PHE:N	1:C:49:PRO:HD2	2.26	0.49
1:B:323:GLU:O	1:B:327:LYS:HG3	2.11	0.49
1:D:345:ARG:NH2	2:I:1:GLC:O1	2.45	0.49
1:A:3:ILE:HD11	1:B:268:ASN:ND2	2.27	0.49
1:C:165:ASP:O	1:D:188:GLY:HA3	2.12	0.49
1:E:262:VAL:HG22	1:F:111:VAL:HG22	1.95	0.49
1:F:342:TYR:CD1	1:F:345:ARG:NH1	2.79	0.49
1:C:259:PHE:CD2	1:D:159:TRP:CD1	3.01	0.49
1:C:86:PHE:HZ	1:D:286:LEU:HD12	1.78	0.49
1:A:179:ILE:C	1:A:179:ILE:HD12	2.32	0.48
1:C:324:ASN:ND2	1:D:115:SER:HA	2.28	0.48
1:C:342:TYR:CD1	1:C:345:ARG:NH1	2.82	0.48
1:D:49:PRO:HA	1:D:76:LEU:HD13	1.95	0.48
1:C:286:LEU:HD13	1:D:86:PHE:HZ	1.78	0.48
1:A:342:TYR:HD1	1:A:345:ARG:HH12	1.56	0.48
1:E:4:GLU:HB2	1:E:7:LYS:HD3	1.92	0.48
1:A:297:ASP:OD2	1:B:19:ASN:HB2	2.13	0.48
1:C:199:LEU:HD23	1:D:134:PRO:HG3	1.96	0.48
1:D:262:VAL:HG23	1:D:330:ILE:HD11	1.95	0.48
1:E:4:GLU:HB3	1:E:7:LYS:HD2	1.93	0.48
1:A:249:PRO:HG2	1:B:130:TRP:NE1	2.28	0.47
1:A:238:THR:OG1	1:C:128:LYS:HE2	2.13	0.47
1:A:342:TYR:CD1	1:A:345:ARG:NH1	2.78	0.47
1:B:7:LYS:HB2	1:B:7:LYS:HE3	1.63	0.47
1:E:180:LYS:HE2	1:E:370:ARG:CG	2.35	0.47
1:E:249:PRO:HG2	1:F:130:TRP:NE1	2.29	0.47
1:B:329:GLU:HG2	1:B:330:ILE:O	2.14	0.47
1:B:342:TYR:CD1	1:B:345:ARG:NH1	2.82	0.47
1:D:7:LYS:HZ2	1:D:7:LYS:CB	2.28	0.47
1:A:73:GLN:CG	1:A:100:TYR:OH	2.56	0.47
1:A:180:LYS:HZ3	1:A:370:ARG:HH11	1.63	0.47
1:C:323:GLU:O	1:C:327:LYS:HG3	2.15	0.47
1:B:90:LEU:CD1	1:B:95:TRP:HZ2	2.26	0.47
1:C:156:TYR:HB2	2:I:1:GLC:H61	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:PRO:HG3	1:D:258:PRO:HA	1.97	0.46
1:C:7:LYS:HE3	1:C:7:LYS:HB2	1.66	0.46
1:E:179:ILE:O	1:E:179:ILE:HD12	2.16	0.46
1:B:171:LYS:HE3	1:B:172:TYR:N	2.29	0.46
1:C:49:PRO:HA	1:C:76:LEU:HD13	1.97	0.46
1:C:246:THR:HG23	1:D:116:LEU:HB3	1.97	0.46
1:E:130:TRP:CD1	1:F:249:PRO:HG2	2.50	0.46
1:C:230:PRO:HA	1:C:233:TRP:CE2	2.51	0.46
1:C:143:LYS:HE3	1:C:143:LYS:HB3	1.71	0.46
1:C:169:ALA:O	1:D:182:VAL:HA	2.15	0.46
1:C:19:ASN:HB2	1:D:297:ASP:OD2	2.16	0.46
1:C:117:ILE:HA	1:D:244:GLY:O	2.16	0.46
1:C:91:TYR:CZ	1:D:306:LYS:HG2	2.51	0.46
1:A:103:LYS:HE2	1:A:103:LYS:HB2	1.57	0.45
1:B:185:ASP:CG	1:B:366:GLN:CG	2.84	0.45
1:D:140:LEU:HD23	1:D:143:LYS:HE2	1.96	0.45
1:A:323:GLU:O	1:A:327:LYS:HG3	2.16	0.45
1:A:127:PRO:HB2	1:A:132:GLU:HG3	1.98	0.45
1:C:150:PHE:HA	1:D:214:ALA:HB1	1.98	0.45
1:D:230:PRO:HA	1:D:233:TRP:CE2	2.52	0.45
1:A:130:TRP:HB3	1:B:195:PHE:CE2	2.51	0.45
1:B:230:PRO:HA	1:B:233:TRP:CE2	2.51	0.45
1:C:168:TYR:CE1	1:D:183:GLY:HA3	2.51	0.45
1:C:65:HIS:NE2	1:D:331:MET:O	2.40	0.45
1:D:4:GLU:HB3	1:D:7:LYS:HG2	1.99	0.45
1:E:244:GLY:CA	1:F:120:LYS:CE	2.95	0.45
1:F:323:GLU:O	1:F:327:LYS:HG3	2.17	0.45
1:C:259:PHE:CD2	1:D:159:TRP:NE1	2.85	0.45
1:D:171:LYS:HA	1:D:171:LYS:HD3	1.57	0.45
1:C:148:LEU:HB2	1:D:225:MET:HE3	1.99	0.45
1:E:227:ILE:HB	1:F:150:PHE:CD2	2.52	0.45
1:C:368:ASN:C	1:C:370:ARG:H	2.20	0.45
1:F:230:PRO:HA	1:F:233:TRP:CE2	2.51	0.45
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.51	0.45
1:E:323:GLU:O	1:E:327:LYS:HG3	2.16	0.45
1:D:331:MET:SD	1:D:341:TRP:HZ2	2.40	0.45
1:E:262:VAL:HG23	1:E:330:ILE:HD11	1.99	0.45
1:F:247:VAL:HG22	1:F:323:GLU:OE1	2.16	0.45
1:C:5:GLU:HA	1:D:273:ASN:OD1	2.17	0.45
1:D:7:LYS:HB2	1:D:7:LYS:HZ2	1.80	0.45
1:E:230:PRO:HA	1:E:233:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:GLU:O	1:D:327:LYS:HG3	2.17	0.44
1:A:347:ALA:HB2	1:A:365:ALA:HB2	1.99	0.44
1:E:227:ILE:HB	1:F:150:PHE:HD2	1.81	0.44
1:A:180:LYS:NZ	1:A:370:ARG:HH11	2.15	0.44
1:F:7:LYS:HB2	1:F:7:LYS:HE3	1.59	0.44
1:C:370:ARG:C	1:C:370:ARG:CD	2.85	0.44
1:A:179:ILE:HD12	1:A:179:ILE:O	2.18	0.44
1:A:68:PHE:HE2	1:B:266:GLY:HA3	1.82	0.44
1:A:214:ALA:HA	1:B:149:MET:HE2	2.00	0.44
1:A:34:ILE:HG13	1:B:276:LEU:HD22	1.99	0.44
1:D:370:ARG:CD	1:D:370:ARG:C	2.85	0.44
1:A:262:VAL:HG22	1:B:111:VAL:HG22	1.99	0.44
1:C:63:TRP:CZ2	2:I:2:GLC:H61	2.53	0.43
1:D:180:LYS:HE2	1:D:180:LYS:CA	2.14	0.43
1:E:4:GLU:O	1:E:7:LYS:HG2	2.18	0.43
1:A:366:GLN:HG3	1:A:370:ARG:HH21	1.84	0.43
1:A:303:VAL:HA	1:B:110:ALA:HA	2.00	0.43
1:C:268:ASN:HB2	1:D:58:PRO:O	2.17	0.43
1:E:231:TRP:CE3	1:F:16:LYS:HE3	2.53	0.43
1:E:68:PHE:HE2	1:F:266:GLY:HA3	1.83	0.43
1:A:150:PHE:HA	1:B:214:ALA:HB1	2.01	0.43
1:A:203:LYS:O	1:B:141:LYS:NZ	2.50	0.43
1:B:185:ASP:N	1:B:185:ASP:OD1	2.45	0.43
1:E:214:ALA:HB1	1:F:150:PHE:HA	2.01	0.43
1:E:263:LEU:O	1:F:109:ILE:HB	2.19	0.43
1:A:273:ASN:OD1	1:B:5:GLU:HA	2.19	0.43
1:A:48:PHE:CD1	1:A:48:PHE:C	2.93	0.43
1:C:221:GLY:O	1:D:122:LEU:HD11	2.19	0.43
1:D:302:ALA:HA	1:D:309:GLU:OE2	2.19	0.43
1:E:225:MET:SD	1:F:127:PRO:HD2	2.59	0.43
1:B:182:VAL:HB	1:B:366:GLN:NE2	2.34	0.42
1:A:122:LEU:HD21	1:A:145:LYS:CE	2.49	0.42
1:C:249:PRO:HB2	1:D:130:TRP:CD1	2.54	0.42
1:E:58:PRO:O	1:F:268:ASN:HB2	2.19	0.42
1:C:284:TYR:CE2	1:D:28:PHE:HA	2.55	0.42
1:D:190:LYS:HE2	1:D:359:ASP:HA	2.01	0.42
1:E:150:PHE:HA	1:F:214:ALA:HB1	2.02	0.42
1:C:303:VAL:HA	1:D:110:ALA:HA	2.01	0.42
1:F:302:ALA:HA	1:F:309:GLU:OE2	2.20	0.42
1:F:52:ALA:HA	1:F:56:ASP:O	2.20	0.42
1:A:180:LYS:CE	1:A:370:ARG:HD3	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:370:ARG:CG	1:F:370:ARG:NH1	2.72	0.42
1:E:179:ILE:C	1:E:179:ILE:HD12	2.40	0.41
1:C:130:TRP:CE2	1:D:249:PRO:HG2	2.55	0.41
1:D:171:LYS:HD3	1:D:172:TYR:H	1.84	0.41
1:E:306:LYS:HG2	1:F:91:TYR:CE1	2.54	0.41
1:E:370:ARG:C	1:E:370:ARG:CD	2.84	0.41
1:A:171:LYS:HB2	1:B:181:ASP:CG	2.40	0.41
1:A:90:LEU:CD1	1:A:95:TRP:HZ2	2.31	0.41
1:C:304:ALA:O	1:D:90:LEU:HA	2.21	0.41
1:C:86:PHE:HA	1:C:89:LYS:HE2	2.03	0.41
1:D:370:ARG:O	1:D:370:ARG:HG3	2.20	0.41
1:E:266:GLY:HA3	1:F:68:PHE:HE2	1.85	0.41
1:E:90:LEU:HB2	1:E:95:TRP:NE1	2.35	0.41
1:A:180:LYS:CE	1:A:370:ARG:CD	2.91	0.41
1:A:238:THR:CG2	1:C:126:PRO:HD2	2.50	0.41
1:C:52:ALA:HA	1:C:56:ASP:O	2.20	0.41
1:A:180:LYS:HZ3	1:A:370:ARG:HD2	1.85	0.41
1:B:331:MET:SD	1:B:341:TRP:HZ2	2.44	0.41
1:E:148:LEU:HB2	1:F:225:MET:HE3	2.01	0.41
1:D:52:ALA:HA	1:D:56:ASP:O	2.20	0.41
1:F:49:PRO:HA	1:F:76:LEU:CD1	2.50	0.41
1:E:52:ALA:HA	1:E:56:ASP:O	2.20	0.41
1:E:153:GLN:HG2	1:F:210:ASP:HA	2.03	0.41
1:A:166:GLY:O	1:B:186:ASN:ND2	2.53	0.41
1:A:123:LEU:HD21	1:A:126:PRO:HA	2.04	0.40
1:A:91:TYR:CE1	1:B:306:LYS:HG2	2.56	0.40
1:B:90:LEU:HB2	1:B:95:TRP:NE1	2.36	0.40
1:D:370:ARG:O	1:D:370:ARG:CG	2.69	0.40
1:E:62:PHE:CZ	1:F:285:LEU:CD2	3.03	0.40
1:A:52:ALA:HA	1:A:56:ASP:O	2.21	0.40
1:D:159:TRP:N	1:D:160:PRO:CD	2.85	0.40
1:C:368:ASN:C	1:C:370:ARG:N	2.74	0.40
1:F:331:MET:SD	1:F:341:TRP:HZ2	2.44	0.40
1:C:312:LEU:HD23	1:C:312:LEU:HA	1.85	0.40
1:C:262:VAL:HG23	1:C:330:ILE:HD11	2.03	0.40
1:C:370:ARG:C	1:C:370:ARG:NH1	2.73	0.40
1:D:27:LYS:HA	1:D:30:LYS:CE	2.51	0.40
1:D:4:GLU:HB3	1:D:7:LYS:CG	2.51	0.40
1:E:110:ALA:HA	1:F:303:VAL:HA	2.02	0.40
1:E:8:LEU:HA	1:E:8:LEU:HD23	1.96	0.40
1:A:79:GLU:HB2	1:A:103:LYS:HE3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:THR:HG23	1:A:132:GLU:H	1.86	0.40
1:E:302:ALA:HA	1:E:309:GLU:OE2	2.22	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:B:247:VAL:CG2	1:E:142:ALA:O[1_566]	2.19	0.01

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	367/419 (88%)	363 (99%)	4 (1%)	0	100	100
1	B	367/419 (88%)	362 (99%)	5 (1%)	0	100	100
1	C	366/419 (87%)	359 (98%)	6 (2%)	1 (0%)	41	74
1	D	366/419 (87%)	361 (99%)	5 (1%)	0	100	100
1	E	366/419 (87%)	359 (98%)	6 (2%)	1 (0%)	41	74
1	F	366/419 (87%)	360 (98%)	4 (1%)	2 (0%)	29	67
All	All	2198/2514 (87%)	2164 (98%)	30 (1%)	4 (0%)	47	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	174	ALA
1	E	174	ALA
1	C	369	ALA
1	F	169	ALA

5.3.2 Protein sidechains ⓘ

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	287/335 (86%)	274 (96%)	13 (4%)	27	63
1	B	287/335 (86%)	276 (96%)	11 (4%)	33	67
1	C	286/335 (85%)	277 (97%)	9 (3%)	40	72
1	D	286/335 (85%)	273 (96%)	13 (4%)	27	63
1	E	286/335 (85%)	279 (98%)	7 (2%)	49	77
1	F	286/335 (85%)	275 (96%)	11 (4%)	33	67
All	All	1718/2010 (86%)	1654 (96%)	64 (4%)	34	68

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	30	LYS
1	A	39	GLU
1	A	73	GLN
1	A	115	SER
1	A	136	LEU
1	A	171	LYS
1	A	176	LYS
1	A	180	LYS
1	A	212	SER
1	A	259	PHE
1	A	278	LYS
1	A	309	GLU
1	B	125	ASN
1	B	136	LEU
1	B	143	LYS
1	B	171	LYS
1	B	179	ILE
1	B	185	ASP
1	B	254	GLN
1	B	259	PHE
1	B	278	LYS

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Mol	Chain	Res	Type
1	B	292	GLU
1	B	370	ARG
1	C	136	LEU
1	C	143	LYS
1	C	176	LYS
1	C	179	ILE
1	C	239	SER
1	C	259	PHE
1	C	292	GLU
1	C	329	GLU
1	C	370	ARG
1	D	7	LYS
1	D	30	LYS
1	D	42	ASP
1	D	136	LEU
1	D	171	LYS
1	D	180	LYS
1	D	208	ASP
1	D	212	SER
1	D	239	SER
1	D	259	PHE
1	D	292	GLU
1	D	309	GLU
1	D	370	ARG
1	E	128	LYS
1	E	136	LEU
1	E	180	LYS
1	E	212	SER
1	E	239	SER
1	E	259	PHE
1	E	370	ARG
1	F	5	GLU
1	F	27	LYS
1	F	136	LEU
1	F	150	PHE
1	F	171	LYS
1	F	212	SER
1	F	254	GLN
1	F	259	PHE
1	F	278	LYS
1	F	309	GLU
1	F	370	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	366	GLN
1	B	125	ASN
1	B	283	ASN
1	C	204	HIS
1	C	254	GLN
1	C	283	ASN
1	F	254	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

12 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	GLC	G	1	2	12,12,12	1.38	2 (16%)	17,17,17	2.04	6 (35%)
2	GLC	G	2	2	11,11,12	0.91	0	15,15,17	2.13	6 (40%)
2	GLC	H	1	2	12,12,12	1.06	2 (16%)	17,17,17	1.80	6 (35%)
2	GLC	H	2	2	11,11,12	0.58	0	15,15,17	1.62	1 (6%)
2	GLC	I	1	2	12,12,12	1.15	1 (8%)	17,17,17	2.24	7 (41%)
2	GLC	I	2	2	11,11,12	0.97	0	15,15,17	1.54	2 (13%)
2	GLC	J	1	2	12,12,12	0.94	0	17,17,17	2.25	9 (52%)
2	GLC	J	2	2	11,11,12	0.72	0	15,15,17	1.58	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	K	1	2	12,12,12	0.75	0	17,17,17	1.34	2 (11%)
2	GLC	K	2	2	11,11,12	0.56	0	15,15,17	1.85	3 (20%)
2	GLC	L	1	2	12,12,12	1.03	1 (8%)	17,17,17	1.64	4 (23%)
2	GLC	L	2	2	11,11,12	0.79	0	15,15,17	2.35	5 (33%)

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	GLC	G	1	2	-	1/2/22/22	0/1/1/1
2	GLC	G	2	2	-	2/2/19/22	0/1/1/1
2	GLC	H	1	2	-	0/2/22/22	0/1/1/1
2	GLC	H	2	2	-	2/2/19/22	0/1/1/1
2	GLC	I	1	2	-	2/2/22/22	0/1/1/1
2	GLC	I	2	2	-	1/2/19/22	0/1/1/1
2	GLC	J	1	2	-	2/2/22/22	0/1/1/1
2	GLC	J	2	2	-	1/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/22/22	0/1/1/1
2	GLC	K	2	2	-	2/2/19/22	0/1/1/1
2	GLC	L	1	2	-	0/2/22/22	0/1/1/1
2	GLC	L	2	2	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	GLC	O1-C1	2.34	1.47	1.39
2	I	1	GLC	O1-C1	2.32	1.47	1.39
2	H	1	GLC	O1-C1	2.09	1.46	1.39
2	G	1	GLC	C4-C5	-2.09	1.48	1.53
2	H	1	GLC	C1-C2	2.07	1.57	1.52
2	L	1	GLC	O1-C1	2.01	1.46	1.39

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	2	GLC	C1-O5-C5	6.41	120.87	112.19
2	H	2	GLC	C1-O5-C5	5.13	119.14	112.19
2	J	1	GLC	C3-C4-C5	-4.67	101.92	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	2	GLC	C1-O5-C5	4.51	118.31	112.19
2	I	1	GLC	C3-C4-C5	-4.45	102.30	110.24
2	J	1	GLC	C1-O5-C5	4.25	121.67	113.66
2	G	2	GLC	C1-O5-C5	4.15	117.82	112.19
2	L	2	GLC	O3-C3-C2	4.14	117.92	109.99
2	G	2	GLC	O3-C3-C2	3.87	117.40	109.99
2	G	1	GLC	C4-C3-C2	-3.86	104.08	110.82
2	K	2	GLC	O5-C5-C6	3.54	112.75	107.20
2	I	1	GLC	O4-C4-C5	3.52	118.05	109.30
2	H	1	GLC	C4-C3-C2	-3.37	104.93	110.82
2	L	1	GLC	C4-C3-C2	-3.36	104.96	110.82
2	G	2	GLC	C2-C3-C4	-3.34	105.12	110.89
2	L	1	GLC	C1-O5-C5	3.28	119.84	113.66
2	I	1	GLC	C4-C3-C2	-3.23	105.18	110.82
2	G	1	GLC	O2-C2-C3	3.13	117.59	110.35
2	I	2	GLC	O5-C1-C2	-3.09	106.01	110.77
2	K	2	GLC	C2-C3-C4	-3.07	105.59	110.89
2	G	1	GLC	O6-C6-C5	-3.02	100.94	111.29
2	J	1	GLC	O4-C4-C5	3.01	116.78	109.30
2	J	2	GLC	O5-C1-C2	-3.01	106.12	110.77
2	I	1	GLC	C1-O5-C5	2.89	119.12	113.66
2	G	1	GLC	C1-O5-C5	2.85	119.04	113.66
2	L	2	GLC	O4-C4-C3	-2.75	103.98	110.35
2	H	1	GLC	C1-O5-C5	2.74	118.83	113.66
2	L	1	GLC	O2-C2-C3	2.73	116.66	110.35
2	J	2	GLC	C1-C2-C3	2.72	113.00	109.67
2	K	1	GLC	O5-C1-C2	2.68	115.07	110.28
2	I	1	GLC	O3-C3-C2	2.65	116.47	110.35
2	I	1	GLC	O2-C2-C3	2.56	116.28	110.35
2	J	1	GLC	C4-C3-C2	-2.56	106.36	110.82
2	K	1	GLC	O2-C2-C1	2.49	114.94	109.16
2	J	1	GLC	O4-C4-C3	2.44	116.00	110.35
2	L	2	GLC	C2-C3-C4	-2.43	106.70	110.89
2	I	1	GLC	O4-C4-C3	2.42	115.94	110.35
2	G	1	GLC	C6-C5-C4	-2.41	107.36	113.00
2	J	1	GLC	O2-C2-C3	2.37	115.83	110.35
2	J	1	GLC	O5-C1-C2	2.36	114.50	110.28
2	G	2	GLC	O4-C4-C5	2.36	115.16	109.30
2	I	2	GLC	O4-C4-C5	2.34	115.12	109.30
2	J	1	GLC	O3-C3-C2	2.28	115.63	110.35
2	J	2	GLC	O3-C3-C2	2.28	114.37	109.99
2	G	1	GLC	C3-C4-C5	-2.25	106.22	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	GLC	O5-C1-C2	2.20	114.21	110.28
2	H	1	GLC	C3-C4-C5	-2.20	106.32	110.24
2	G	2	GLC	O2-C2-C3	2.12	114.39	110.14
2	H	1	GLC	O2-C2-C1	2.09	114.01	109.16
2	J	1	GLC	O5-C5-C4	2.07	113.46	109.69
2	H	1	GLC	O5-C5-C6	2.07	111.58	106.44
2	L	2	GLC	O5-C5-C6	2.04	110.40	107.20
2	J	2	GLC	C1-O5-C5	2.03	114.95	112.19
2	J	2	GLC	O2-C2-C3	-2.03	106.06	110.14
2	L	1	GLC	O5-C5-C4	-2.02	106.03	109.69
2	G	2	GLC	C3-C4-C5	-2.00	106.67	110.24

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1	GLC	O5-C5-C6-O6
2	J	1	GLC	O5-C5-C6-O6
2	K	2	GLC	O5-C5-C6-O6
2	H	2	GLC	O5-C5-C6-O6
2	G	2	GLC	O5-C5-C6-O6
2	I	1	GLC	C4-C5-C6-O6
2	K	2	GLC	C4-C5-C6-O6
2	J	1	GLC	C4-C5-C6-O6
2	G	2	GLC	C4-C5-C6-O6
2	L	2	GLC	O5-C5-C6-O6
2	H	2	GLC	C4-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6
2	L	2	GLC	C4-C5-C6-O6
2	G	1	GLC	O5-C5-C6-O6
2	J	2	GLC	O5-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 26 short contacts:

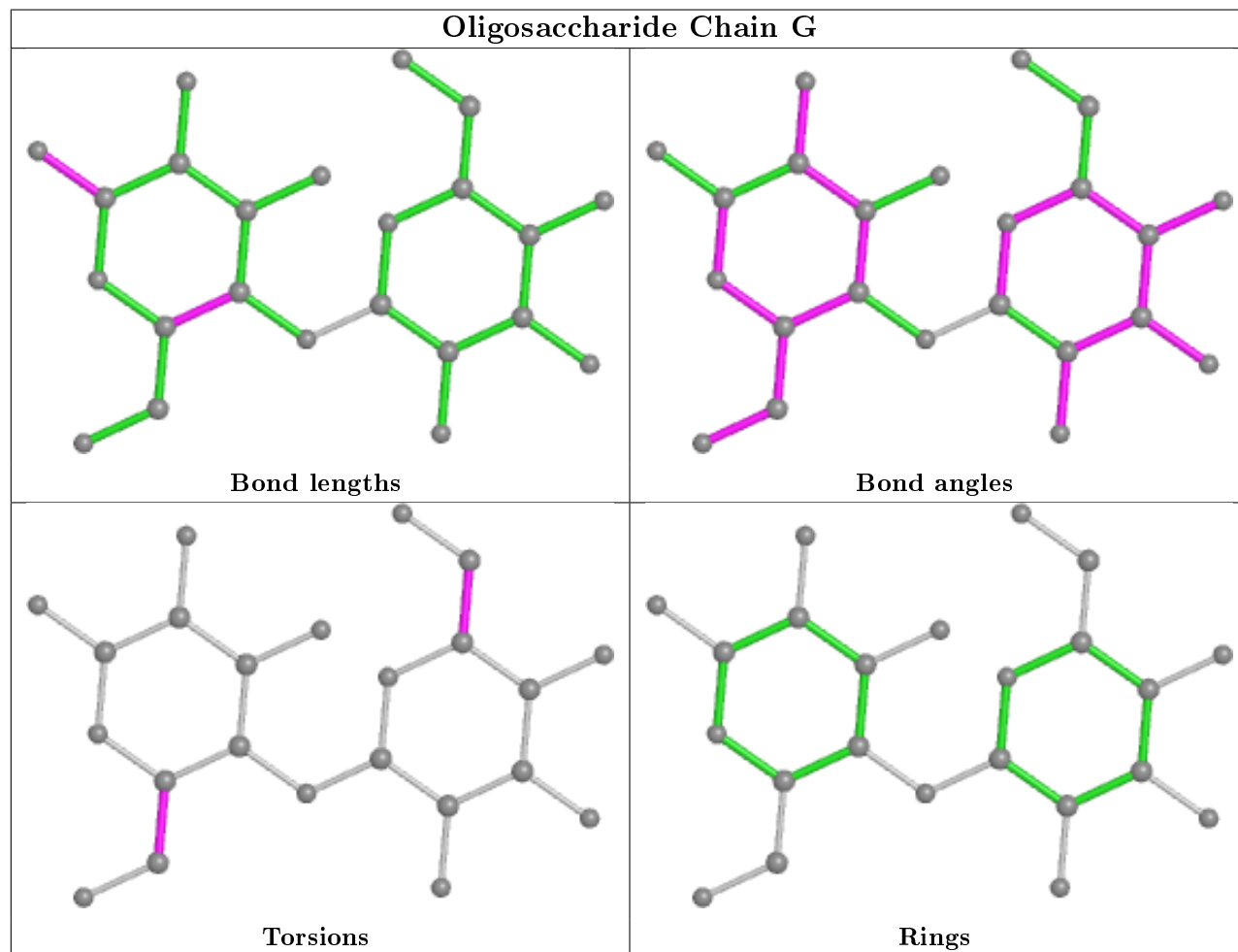
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	GLC	3	0
2	H	1	GLC	4	0
2	J	1	GLC	5	0
2	L	1	GLC	3	0
2	I	2	GLC	2	0

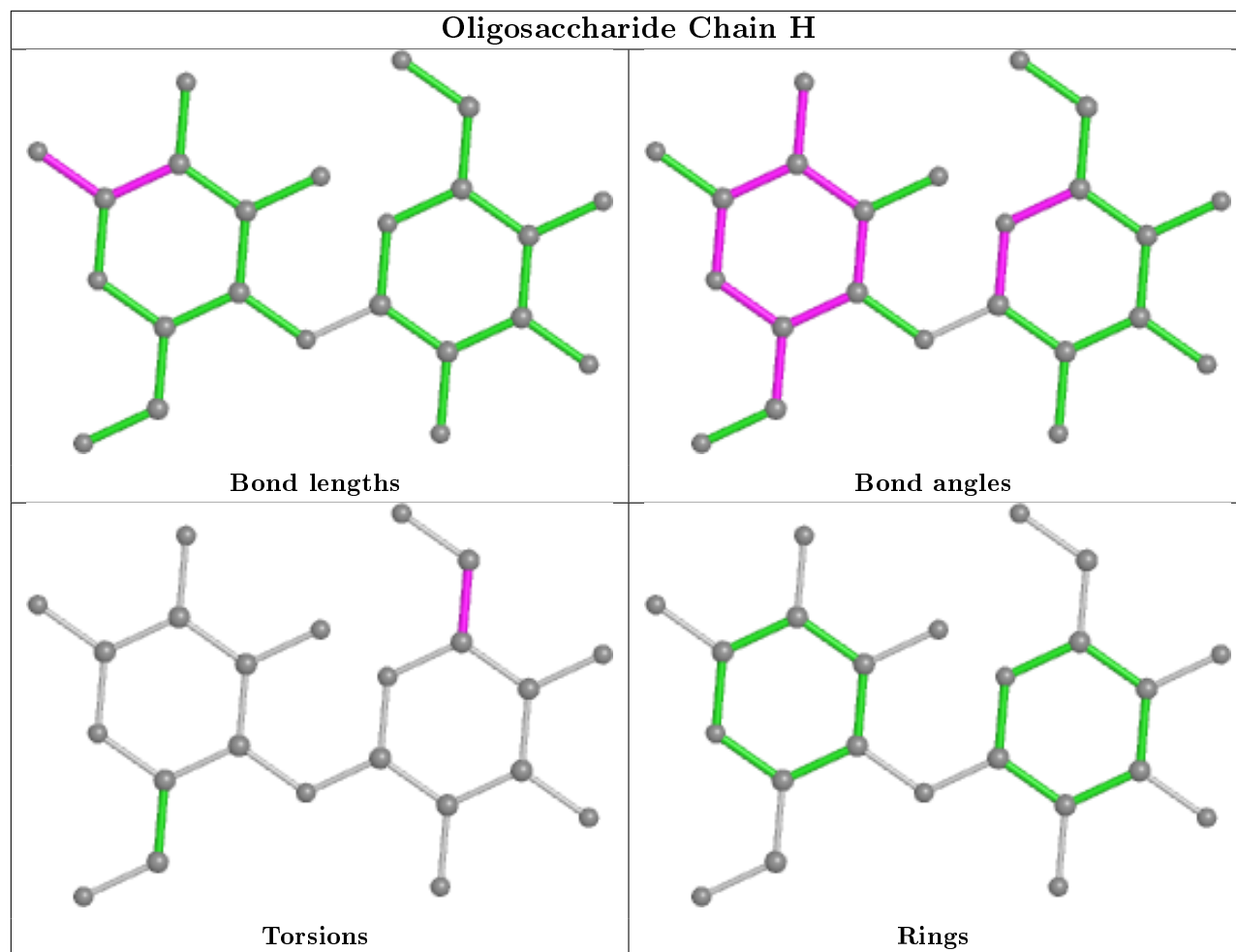
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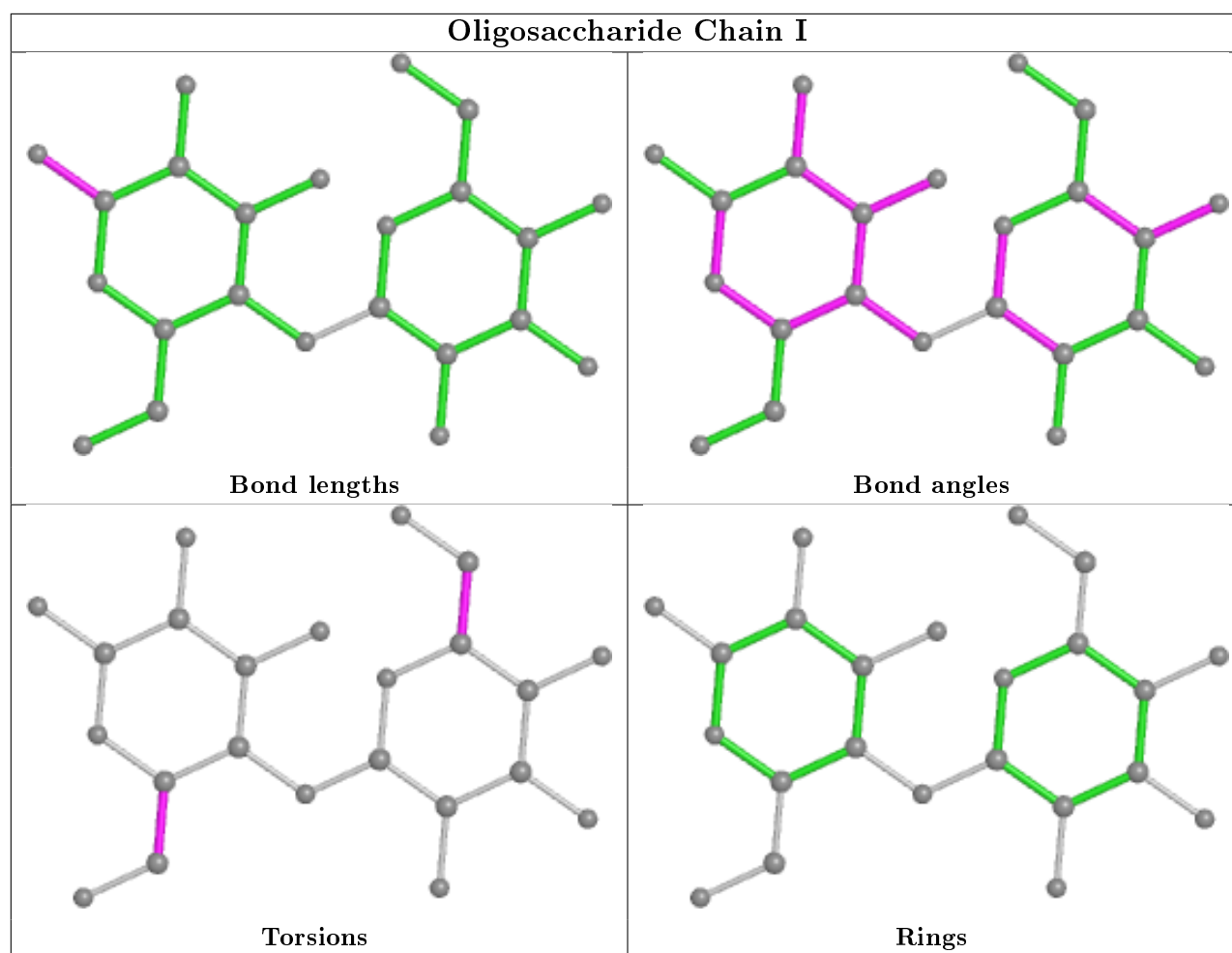
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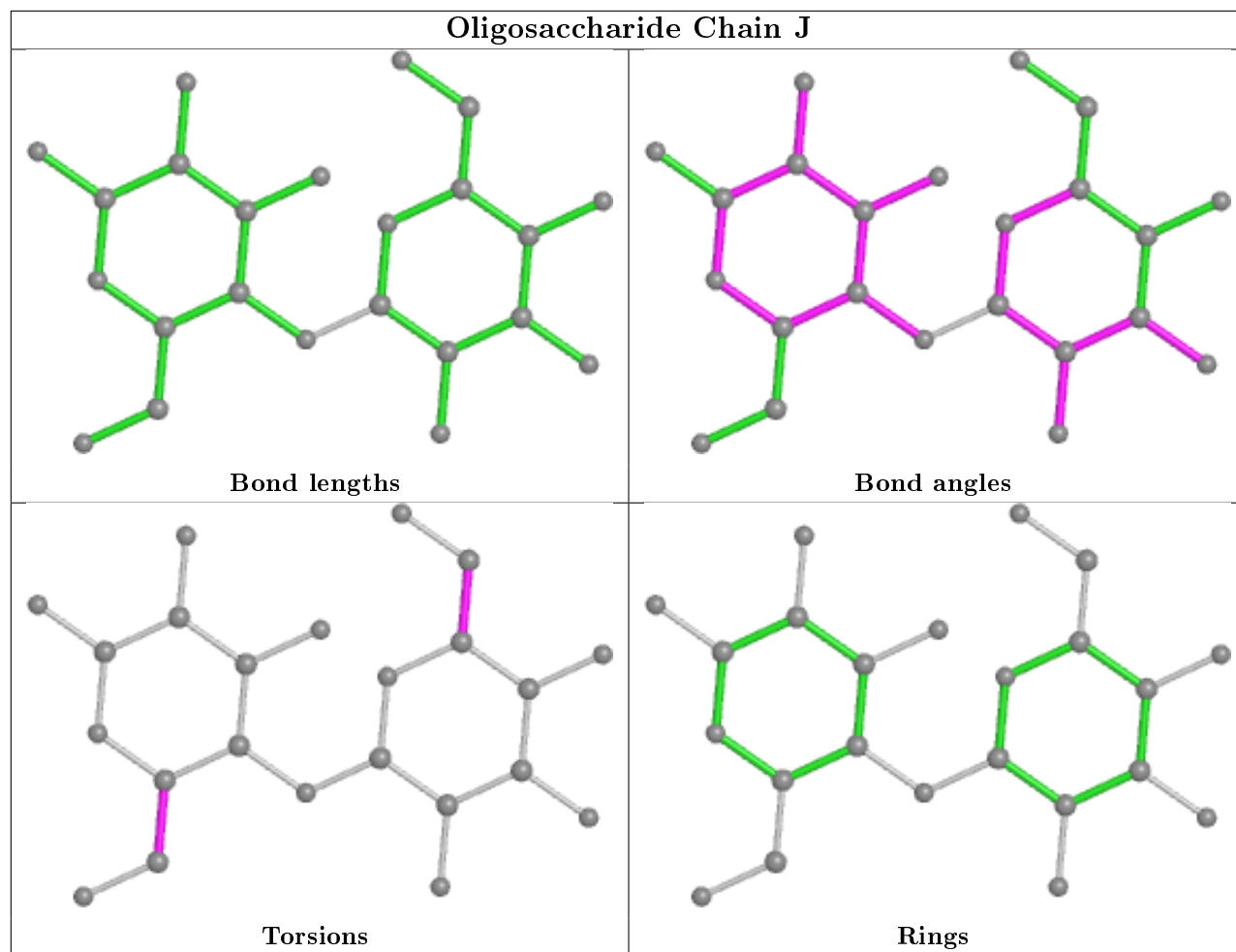
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	GLC	5	0
2	K	1	GLC	4	0

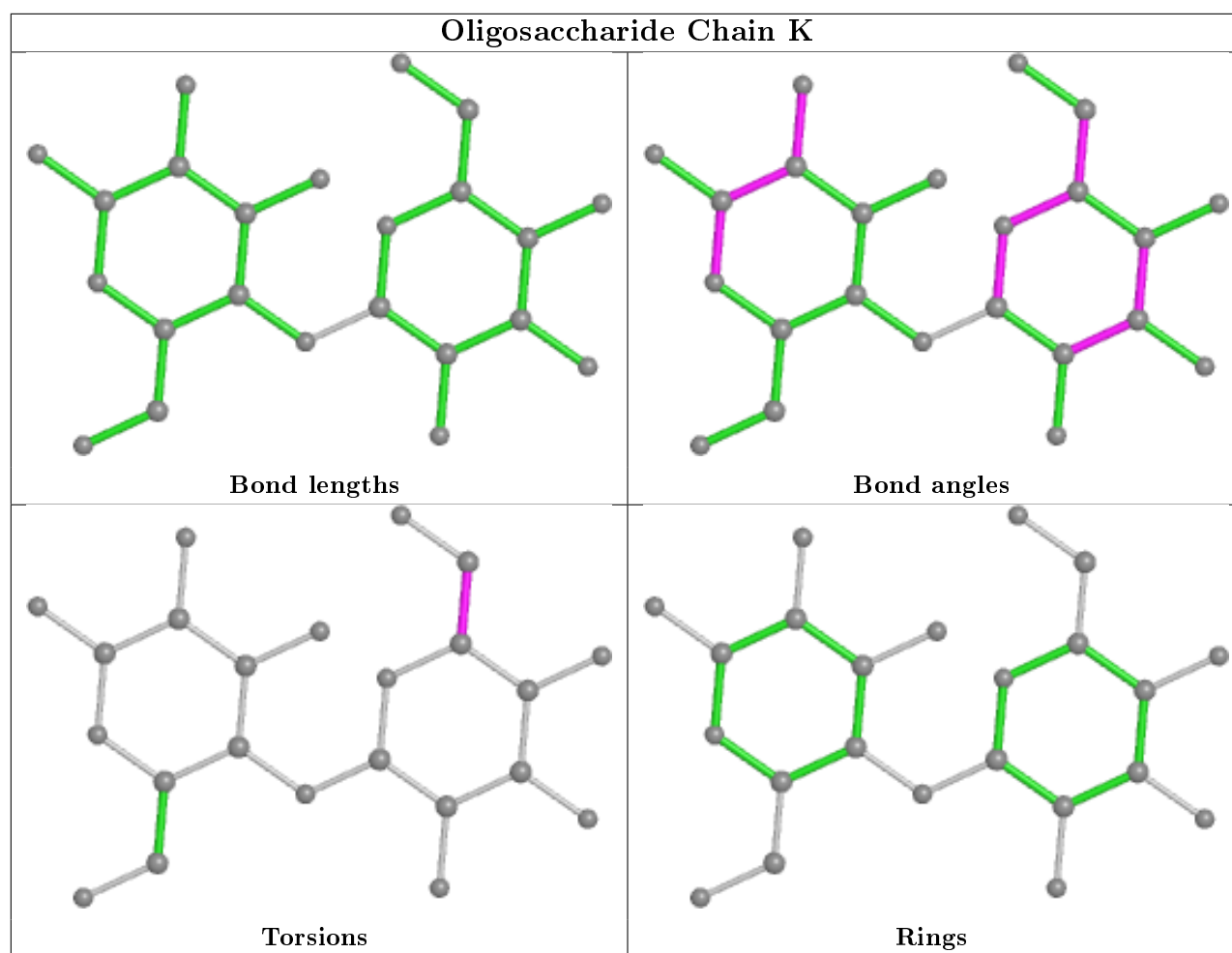
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

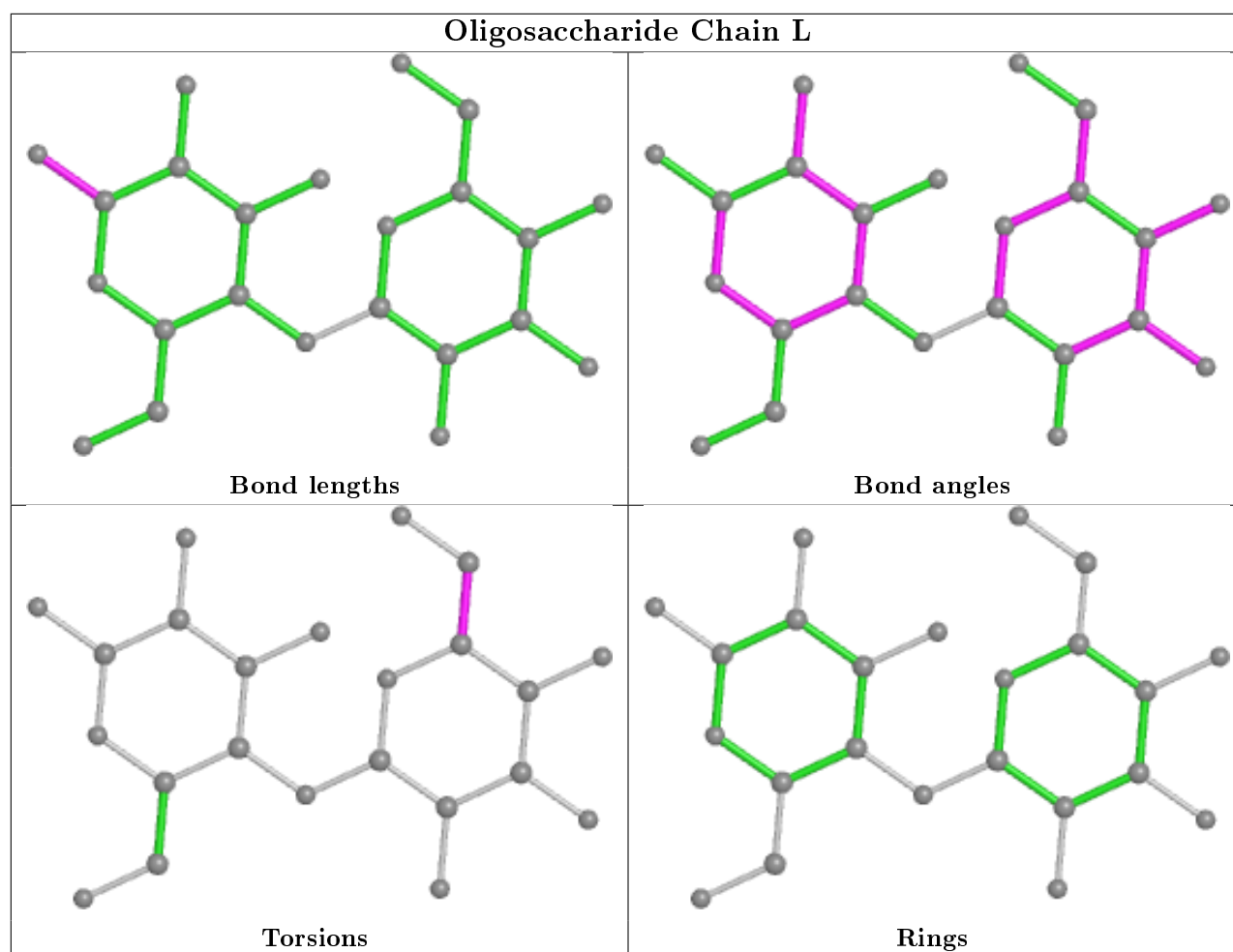












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th 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(Å²)	Q<0.9
1	A	369/419 (88%)	0.10	12 (3%)	46	30	66, 106, 175, 204	0
1	B	369/419 (88%)	0.23	16 (4%)	35	22	59, 102, 184, 227	0
1	C	368/419 (87%)	0.63	37 (10%)	7	4	72, 144, 215, 256	0
1	D	368/419 (87%)	0.63	41 (11%)	5	3	68, 147, 212, 239	0
1	E	368/419 (87%)	0.39	30 (8%)	11	6	48, 108, 237, 283	0
1	F	368/419 (87%)	0.38	27 (7%)	15	9	50, 121, 247, 292	0
All	All	2210/2514 (87%)	0.39	163 (7%)	14	8	48, 120, 216, 292	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	117	ILE	9.0
1	C	233	TRP	8.5
1	C	134	PRO	8.3
1	E	126	PRO	7.8
1	E	146	SER	7.6
1	D	34	ILE	7.3
1	F	218	PHE	7.2
1	E	142	ALA	6.5
1	C	224	ALA	6.5
1	E	123	LEU	6.5
1	C	232	ALA	6.1
1	C	222	GLU	5.7
1	B	3	ILE	5.3
1	F	284	TYR	5.2
1	D	147	ALA	5.2
1	F	256	SER	5.1
1	F	233	TRP	5.1
1	D	21	LEU	5.1
1	E	114	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	232	ALA	4.8
1	F	223	THR	4.8
1	D	309	GLU	4.6
1	E	121	ASP	4.6
1	D	121	ASP	4.6
1	F	240	ALA	4.5
1	E	119	ASN	4.5
1	B	34	ILE	4.5
1	E	147	ALA	4.4
1	E	144	GLY	4.4
1	D	118	TYR	4.3
1	A	284	TYR	4.3
1	E	145	LYS	4.3
1	A	277	ALA	4.2
1	F	231	TRP	4.1
1	F	228	ASN	4.1
1	E	158	THR	4.0
1	E	122	LEU	4.0
1	F	222	GLU	4.0
1	E	125	ASN	3.9
1	D	11	TRP	3.9
1	C	225	MET	3.9
1	D	286	LEU	3.8
1	E	116	LEU	3.8
1	C	219	ASN	3.8
1	C	286	LEU	3.8
1	D	36	VAL	3.7
1	E	124	PRO	3.7
1	F	313	ALA	3.7
1	E	127	PRO	3.7
1	E	149	MET	3.7
1	E	148	LEU	3.6
1	C	221	GLY	3.6
1	A	276	LEU	3.6
1	F	286	LEU	3.6
1	D	129	THR	3.6
1	C	10	ILE	3.5
1	F	243	TYR	3.5
1	D	19	ASN	3.5
1	C	300	LEU	3.5
1	D	145	LYS	3.4
1	C	157	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	28	PHE	3.4
1	F	285	LEU	3.3
1	F	214	ALA	3.3
1	C	309	GLU	3.3
1	D	244	GLY	3.3
1	B	280	PHE	3.2
1	C	230	PRO	3.2
1	D	222	GLU	3.2
1	D	143	LYS	3.2
1	D	105	ILE	3.2
1	E	113	ALA	3.2
1	D	282	GLU	3.2
1	B	130	TRP	3.1
1	D	142	ALA	3.1
1	F	356	GLN	3.1
1	A	59	ASP	3.1
1	A	256	SER	3.1
1	C	16	LYS	3.1
1	D	128	LYS	3.0
1	C	35	LYS	3.0
1	C	226	THR	3.0
1	E	3	ILE	3.0
1	F	221	GLY	2.9
1	C	138	LYS	2.9
1	C	148	LEU	2.9
1	C	301	GLY	2.9
1	C	227	ILE	2.9
1	D	40	HIS	2.9
1	C	283	ASN	2.9
1	D	261	GLY	2.9
1	A	28	PHE	2.9
1	C	299	PRO	2.9
1	B	304	ALA	2.9
1	D	134	PRO	2.8
1	C	249	PRO	2.8
1	D	223	THR	2.8
1	B	60	ILE	2.8
1	E	143	LYS	2.8
1	F	227	ILE	2.8
1	B	30	LYS	2.8
1	B	127	PRO	2.8
1	E	130	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	4	GLU	2.7
1	C	111	VAL	2.7
1	B	107	TYR	2.6
1	D	76	LEU	2.6
1	B	6	GLY	2.6
1	E	34	ILE	2.6
1	E	150	PHE	2.6
1	F	291	LEU	2.5
1	D	111	VAL	2.5
1	C	199	LEU	2.5
1	E	161	LEU	2.5
1	D	33	GLY	2.5
1	D	80	ILE	2.5
1	A	34	ILE	2.5
1	D	16	LYS	2.4
1	E	140	LEU	2.4
1	F	28	PHE	2.4
1	D	107	TYR	2.4
1	C	291	LEU	2.4
1	A	105	ILE	2.4
1	C	105	ILE	2.4
1	C	136	LEU	2.4
1	A	301	GLY	2.3
1	F	225	MET	2.3
1	B	118	TYR	2.3
1	D	173	ALA	2.3
1	A	324	ASN	2.3
1	F	235	ASN	2.3
1	F	246	THR	2.3
1	D	78	ALA	2.3
1	C	170	PHE	2.3
1	C	114	LEU	2.3
1	D	232	ALA	2.3
1	D	236	ILE	2.3
1	D	48	PHE	2.3
1	E	159	TRP	2.3
1	E	133	ILE	2.3
1	F	311	GLU	2.2
1	D	226	THR	2.2
1	C	369	ALA	2.2
1	A	224	ALA	2.2
1	C	348	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	207	ALA	2.2
1	B	35	LYS	2.2
1	C	80	ILE	2.1
1	D	61	ILE	2.1
1	B	25	GLY	2.1
1	D	299	PRO	2.1
1	E	60	ILE	2.1
1	A	280	PHE	2.1
1	F	306	LYS	2.1
1	D	234	SER	2.1
1	C	281	LEU	2.0
1	B	11	TRP	2.0
1	F	248	LEU	2.0
1	D	239	SER	2.0
1	C	280	PHE	2.0
1	B	21	LEU	2.0
1	B	36	VAL	2.0
1	C	211	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

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, 95th 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.

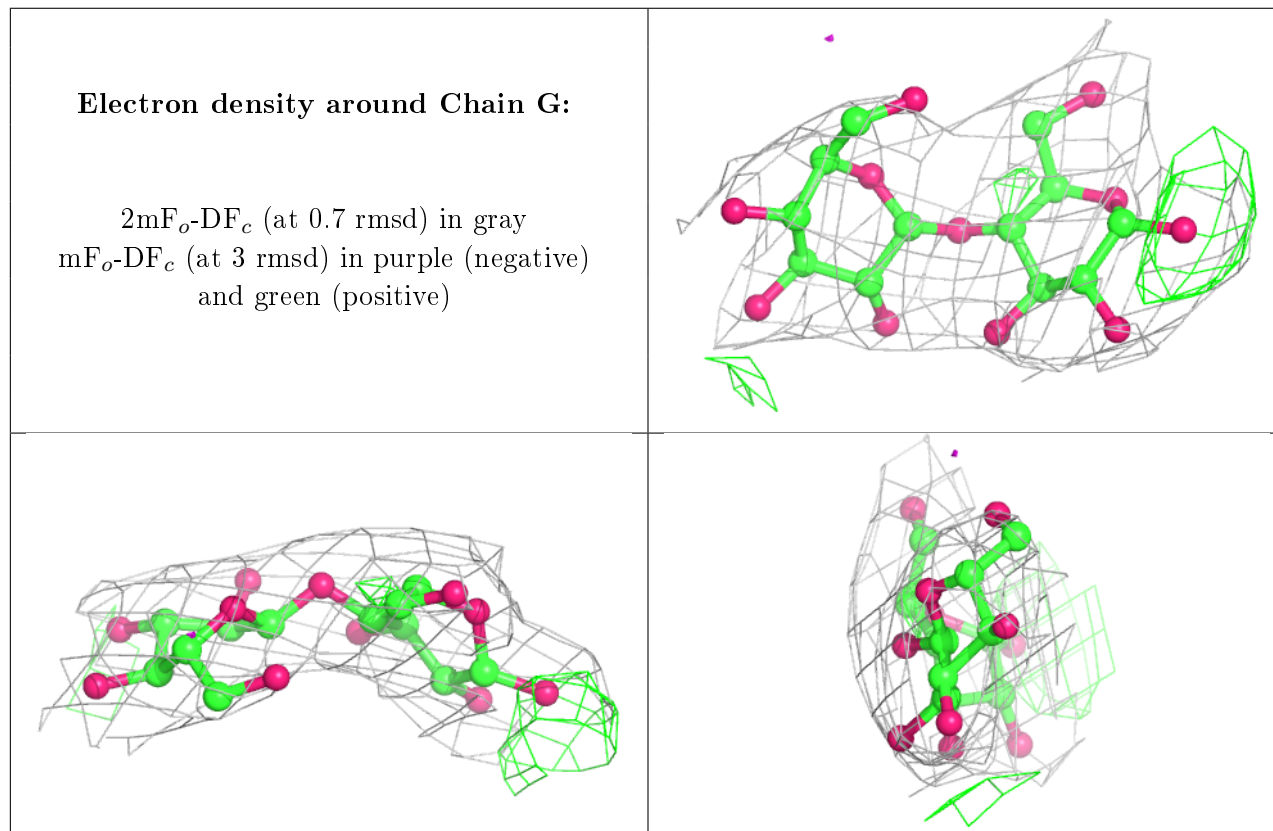
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	I	2	11/12	0.66	0.29	113,157,169,173	0
2	GLC	I	1	12/12	0.79	0.20	99,115,122,131	0
2	GLC	J	1	12/12	0.80	0.19	104,110,118,135	0
2	GLC	J	2	11/12	0.84	0.27	124,165,191,204	0
2	GLC	G	1	12/12	0.87	0.25	55,73,80,80	0
2	GLC	L	1	12/12	0.90	0.30	54,63,74,78	0
2	GLC	K	2	11/12	0.91	0.21	113,129,140,146	0
2	GLC	H	1	12/12	0.93	0.19	69,80,94,100	0
2	GLC	H	2	11/12	0.94	0.26	88,99,110,112	0
2	GLC	K	1	12/12	0.95	0.16	68,78,95,112	0

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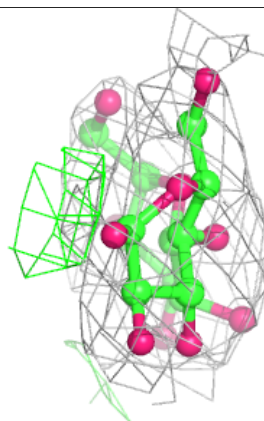
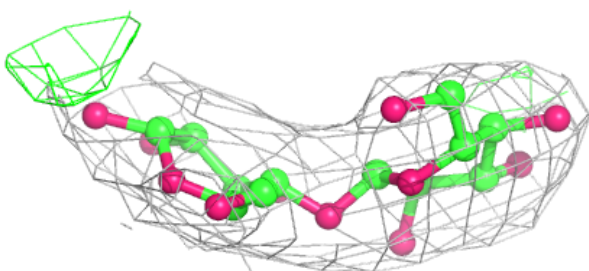
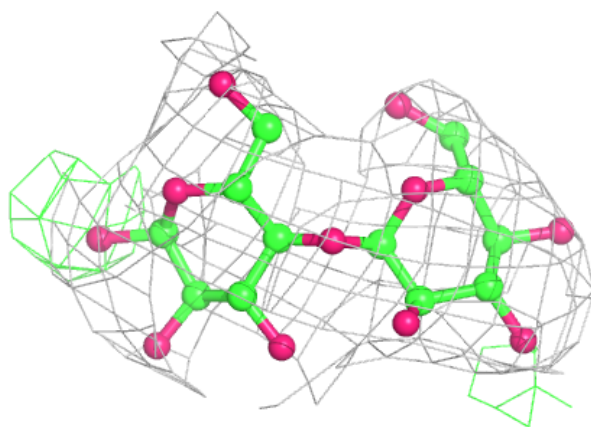
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	G	2	11/12	0.97	0.19	62,73,88,90	0
2	GLC	L	2	11/12	0.98	0.24	57,65,69,71	0

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.

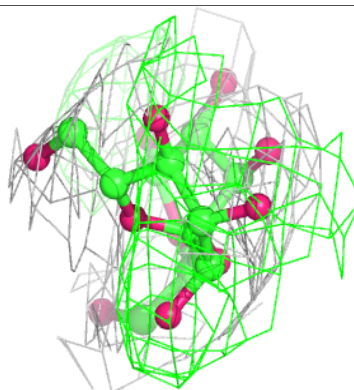
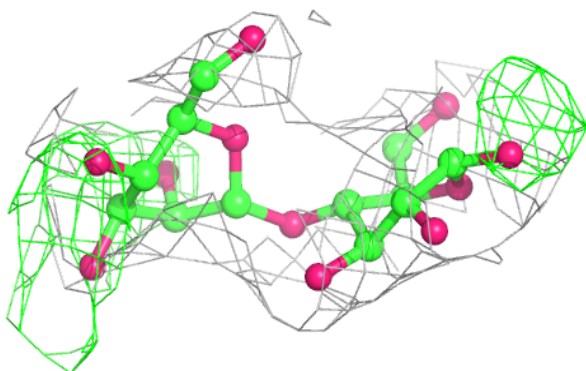
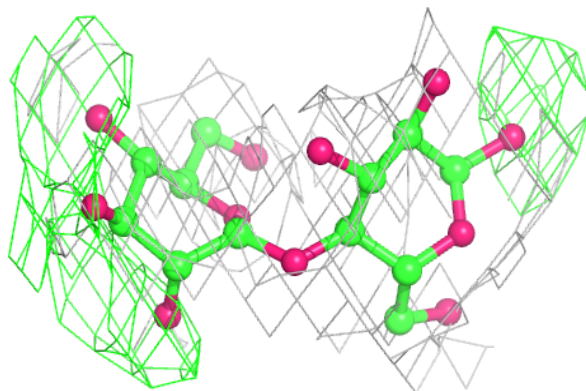


Electron density around Chain H:

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

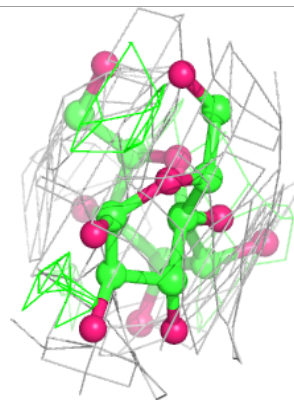
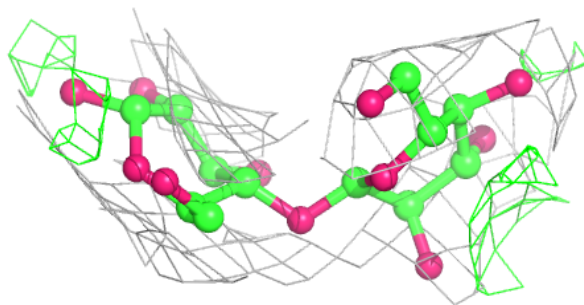
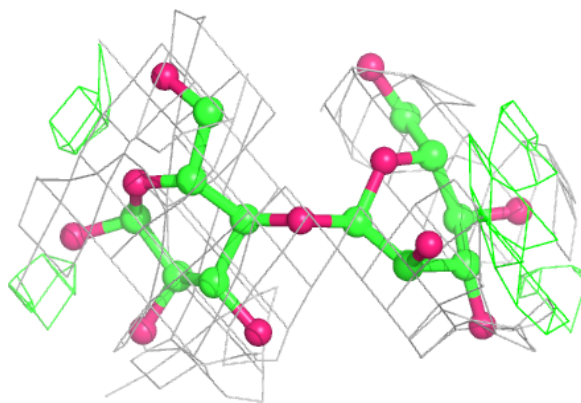
**Electron density around Chain I:**

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



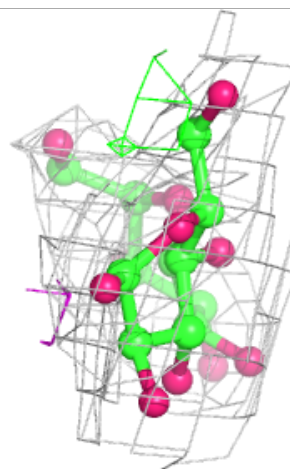
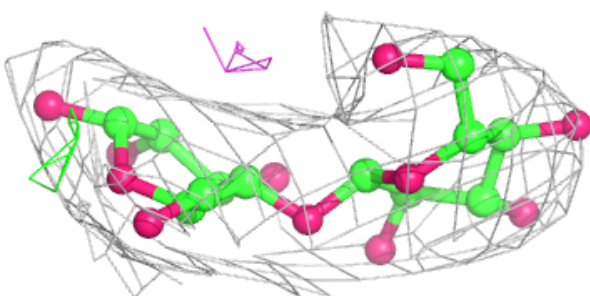
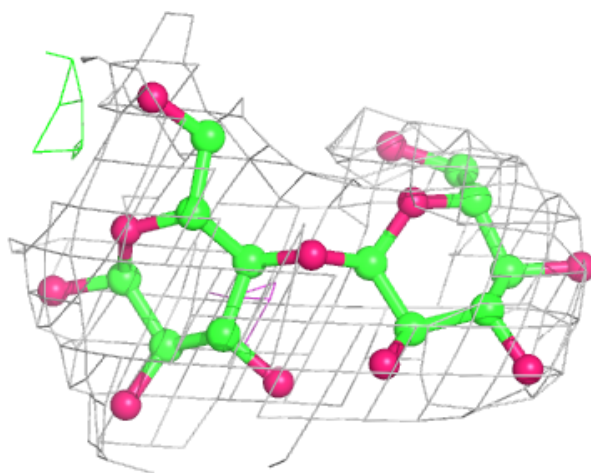
Electron density around Chain J:

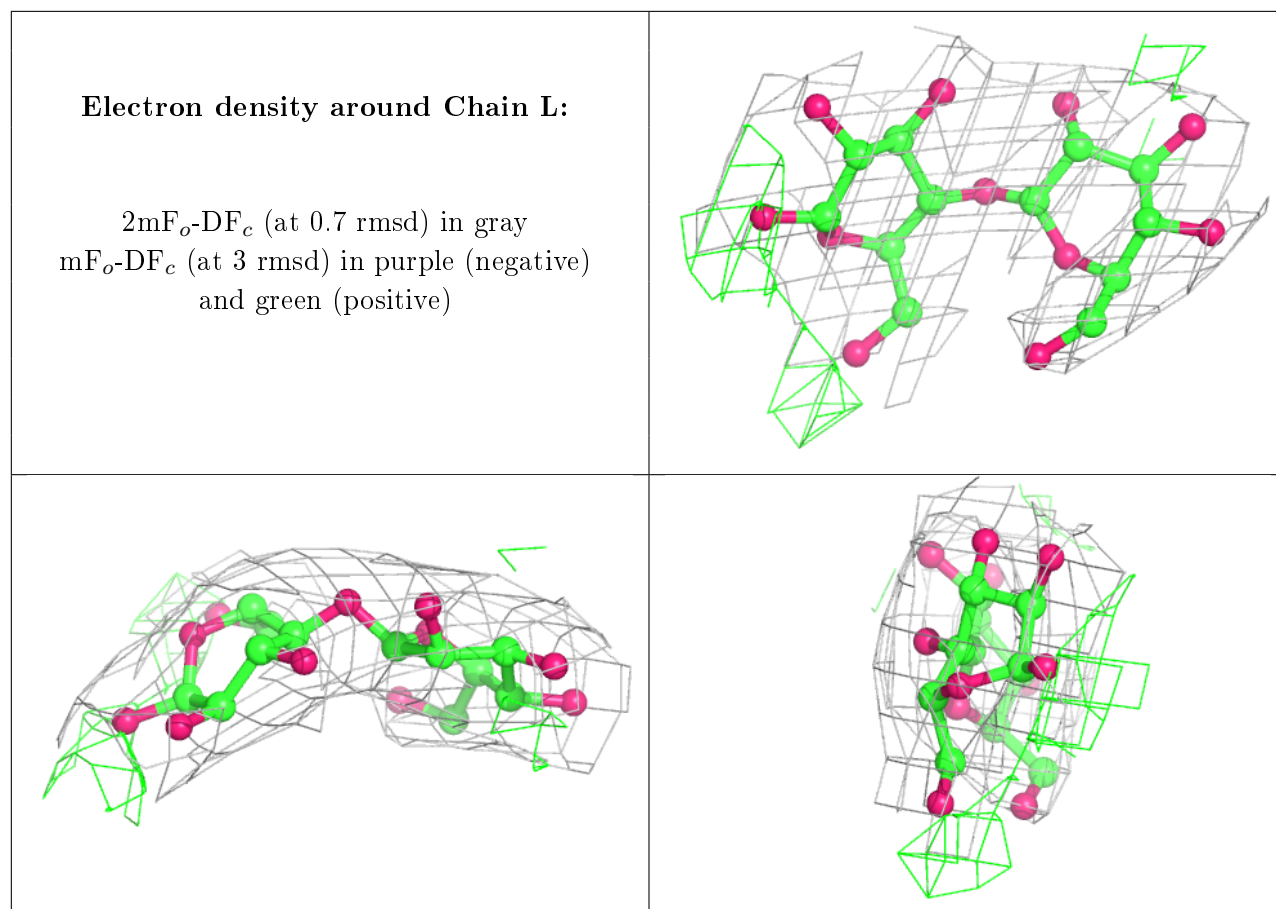
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.