



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 1, 2025 – 10:24 AM JST

PDB ID : 9M73 / pdb_00009m73
Title : Crystal structure of MBP-fused BIL1/BZR1 (21-104) in complex with double-stranded DNA containing CACATATGTG
Authors : Shohei, N.; Masaru, T.; Takuya, M.
Deposited on : 2025-03-09
Resolution : 2.31 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

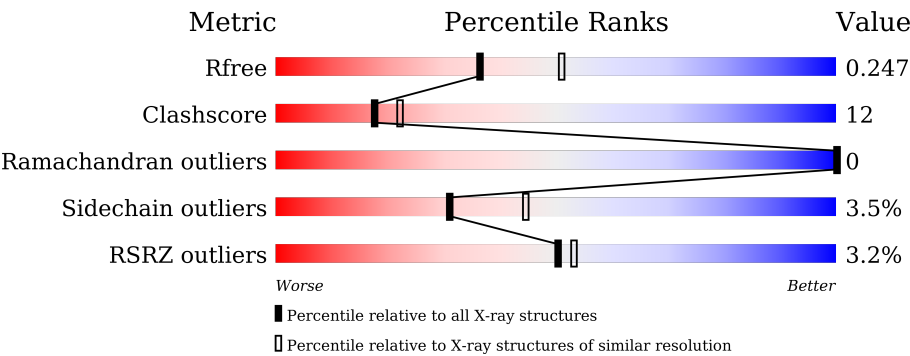
MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

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 2.31 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.





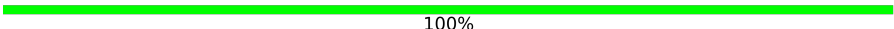



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

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 $\leq 5\%$. 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	453	<div><div>2%</div><div>76%</div><div>19%</div><div>• •</div></div>
1	B	453	<div><div>2%</div><div>79%</div><div>17%</div><div>• •</div></div>
1	C	453	<div><div>2%</div><div>78%</div><div>17%</div><div>• •</div></div>
1	D	453	<div><div>7%</div><div>66%</div><div>29%</div><div>• •</div></div>
2	E	15	<div><div>73%</div><div>27%</div></div>
2	F	15	<div><div>33%</div><div>67%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	15	 87%13%
2	H	15	 73%27%
3	J	2	 100%
3	K	2	 50%50%
3	L	2	 50%50%
3	M	2	 50%50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15105 atoms, of which 30 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 Maltodextrin-binding protein, Protein BRASSINAZOLE-RESISTANT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	436	Total	C	N	O	S	0	0	0
			3394	2166	581	639	8			
1	D	436	Total	C	N	O	S	0	0	0
			3394	2166	581	639	8			
1	A	437	Total	C	N	O	S	0	0	0
			3402	2171	582	640	9			
1	B	436	Total	C	N	O	S	0	0	0
			3394	2166	581	639	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-348	MET	-	initiating methionine	UNP A0A4P1LXE0
C	-266	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
C	-265	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
C	-176	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
C	-175	ALA	ASN	engineered mutation	UNP A0A4P1LXE0
C	-109	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
C	11	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
C	14	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
C	15	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
D	-348	MET	-	initiating methionine	UNP A0A4P1LXE0
D	-266	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
D	-265	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
D	-176	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
D	-175	ALA	ASN	engineered mutation	UNP A0A4P1LXE0
D	-109	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
D	11	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
D	14	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
D	15	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
A	-348	MET	-	initiating methionine	UNP A0A4P1LXE0
A	-266	ALA	ASP	engineered mutation	UNP A0A4P1LXE0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-265	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
A	-176	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
A	-175	ALA	ASN	engineered mutation	UNP A0A4P1LXE0
A	-109	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
A	11	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
A	14	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
A	15	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
B	-348	MET	-	initiating methionine	UNP A0A4P1LXE0
B	-266	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
B	-265	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
B	-176	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
B	-175	ALA	ASN	engineered mutation	UNP A0A4P1LXE0
B	-109	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
B	11	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
B	14	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
B	15	ALA	ASP	engineered mutation	UNP A0A4P1LXE0

- Molecule 2 is a DNA chain called E-box(CATATG)-containing DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	15	Total	C	N	O	P	0	0	0
			305	148	56	87	14			
2	H	15	Total	C	N	O	P	0	0	0
			305	148	56	87	14			
2	E	15	Total	C	N	O	P	0	0	0
			305	148	56	87	14			
2	F	15	Total	C	N	O	P	0	0	0
			305	148	56	87	14			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	M	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	28	Total	O	0	0
			28	28		
5	D	6	Total	O	0	0
			6	6		
5	G	3	Total	O	0	0
			3	3		

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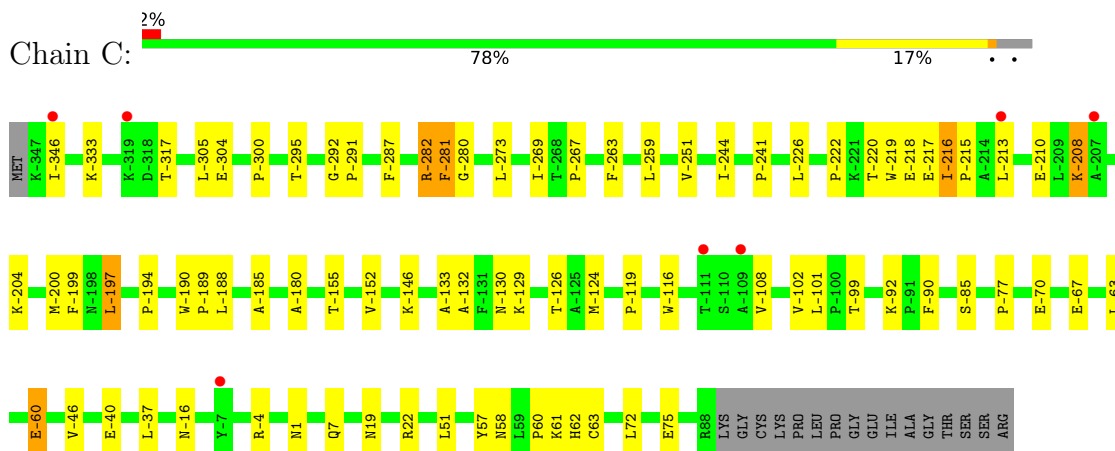
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	5	Total 5	O 5	0	0
5	A	35	Total 35	O 35	0	0
5	B	69	Total 69	O 69	0	0
5	E	2	Total 2	O 2	0	0
5	F	11	Total 11	O 11	0	0

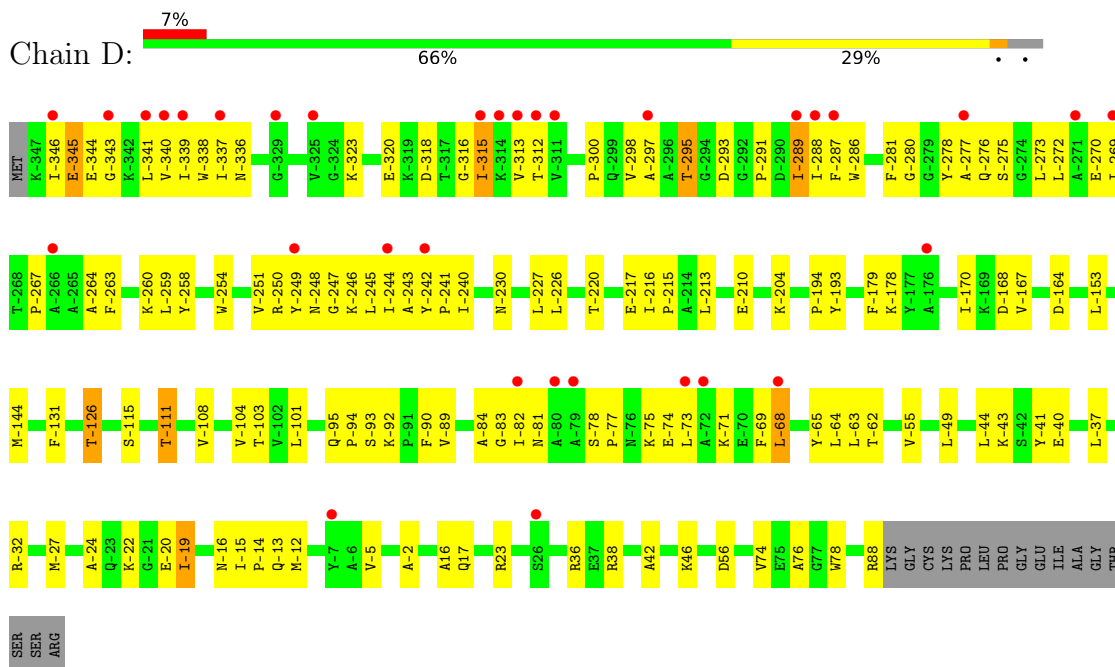
3 Residue-property plots

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.

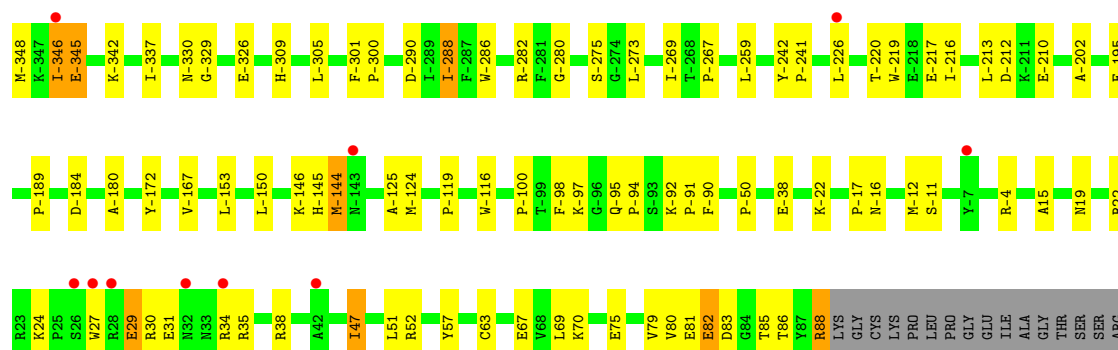
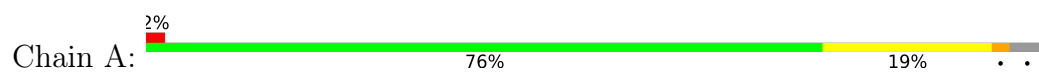
- Molecule 1: Maltodextrin-binding protein,Protein BRASSINAZOLE-RESISTANT 1



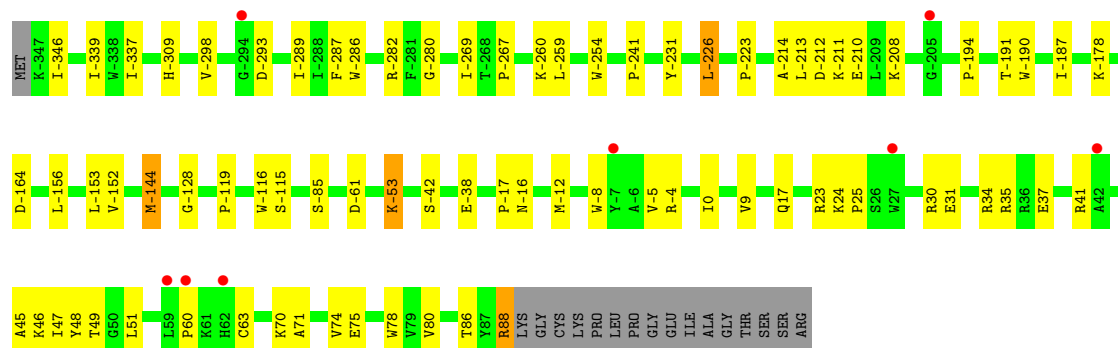
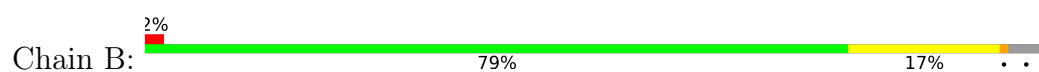
- Molecule 1: Maltodextrin-binding protein,Protein BRASSINAZOLE-RESISTANT 1



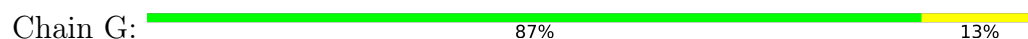
- Molecule 1: Maltodextrin-binding protein,Protein BRASSINAZOLE-RESISTANT 1



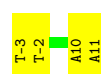
- Molecule 1: Maltodextrin-binding protein, Protein BRASSINAZOLE-RESISTANT 1



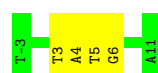
- Molecule 2: E-box(CATATG)-containing DNA




- Molecule 2: E-box(CATATG)-containing DNA

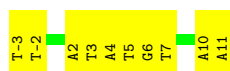


- Molecule 2: E-box(CATATG)-containing DNA



- Molecule 2: E-box(CATATG)-containing DNA

Chain F:  33% 67%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:  100%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:  50% 50%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:  50% 50%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain M:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.85Å 92.60Å 111.77Å 90.00° 100.32° 90.00°	Depositor
Resolution (Å)	43.62 – 2.31 43.62 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.62-2.31) 99.9 (43.62-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.18_3855	Depositor
R, R_{free}	0.205 , 0.245 0.207 , 0.247	Depositor DCC
R_{free} test set	4570 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15105	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4325e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, EDO

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	0.24	1/3481 (0.0%)	0.38	0/4723
1	B	0.30	0/3473	0.40	0/4713
1	C	0.42	3/3473 (0.1%)	0.40	2/4713 (0.0%)
1	D	0.22	0/3473	0.37	0/4713
2	E	0.40	0/342	0.62	0/526
2	F	0.37	0/342	0.56	0/526
2	G	0.29	0/342	0.57	0/526
2	H	0.34	0/342	0.56	0/526
All	All	0.31	4/15268 (0.0%)	0.41	2/20966 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	-180	ALA	C-O	-8.38	1.17	1.23
1	C	-282	ARG	C-O	-5.74	1.16	1.24
1	C	-281	PHE	C-O	-5.25	1.17	1.24
1	A	-216	ILE	CA-CB	5.05	1.57	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	-281	PHE	N-CA-C	5.05	116.87	111.36
1	C	-108	VAL	N-CA-C	5.02	119.79	109.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3402	0	3374	76	0
1	B	3394	0	3365	62	0
1	C	3394	0	3365	59	0
1	D	3394	0	3365	150	0
2	E	305	0	172	6	0
2	F	305	0	172	9	0
2	G	305	0	172	1	0
2	H	305	0	172	2	0
3	J	23	0	21	0	0
3	K	23	0	21	1	0
3	L	23	0	21	0	0
3	M	23	0	21	1	0
4	A	4	6	6	3	0
4	B	12	18	18	0	0
4	C	4	6	6	0	0
5	A	35	0	0	1	0
5	B	69	0	0	6	0
5	C	28	0	0	1	0
5	D	6	0	0	1	0
5	E	2	0	0	0	0
5	F	11	0	0	0	0
5	G	3	0	0	0	0
5	H	5	0	0	0	0
All	All	15075	30	14271	355	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (355) 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:D:-263:PHE:HA	1:D:-260:LYS:HD2	1.30	1.13
1:C:-269:ILE:HG22	1:C:-267:PRO:HD3	1.32	1.09
1:D:-249:TYR:HB3	1:D:-244:ILE:HD11	1.35	1.09
1:A:-345:GLU:HG3	1:A:-342:LYS:HD3	1.33	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ARG:HH11	1:B:88:ARG:HB3	1.23	1.03
1:C:-346:ILE:CG2	1:C:-77:PRO:HD2	1.97	0.95
1:D:-339:ILE:HG12	1:D:-289:ILE:HG13	1.47	0.95
1:D:-269:ILE:HG22	1:D:-267:PRO:HD3	1.49	0.94
1:C:-346:ILE:HG21	1:C:-77:PRO:HD2	1.48	0.94
1:D:-259:LEU:HD11	1:D:-63:LEU:HD13	1.52	0.92
1:D:-346:ILE:HD13	1:D:-77:PRO:HG3	1.57	0.87
1:D:-315:ILE:HD12	1:D:-73:LEU:HD21	1.56	0.86
1:B:30:ARG:HD2	1:B:34:ARG:HH22	1.40	0.85
1:A:31:GLU:OE2	1:A:35:ARG:HD2	1.76	0.85
1:A:80:VAL:HG12	1:A:86:THR:HG23	1.59	0.84
1:D:-341:LEU:HB2	1:D:-313:VAL:HG22	1.61	0.82
1:D:-242:TYR:CE2	1:D:-68:LEU:HB3	2.13	0.82
1:B:45:ALA:O	1:B:49:THR:HG23	1.81	0.81
1:D:-344:GLU:HG3	1:D:-77:PRO:HB2	1.61	0.81
1:D:-248:ASN:O	1:D:-248:ASN:ND2	2.13	0.81
1:D:-249:TYR:CB	1:D:-244:ILE:HD11	2.11	0.80
1:A:-220:THR:HG22	1:A:-217:GLU:OE1	1.80	0.80
1:D:-280:GLY:HA3	1:D:-16:ASN:O	1.82	0.79
1:A:29:GLU:OE2	1:A:29:GLU:HA	1.82	0.79
1:D:-94:PRO:HG2	1:D:-92:LYS:HE3	1.64	0.79
1:D:-341:LEU:CB	1:D:-313:VAL:HG22	2.12	0.78
1:A:-269:ILE:HG22	1:A:-267:PRO:HD3	1.64	0.78
1:A:-220:THR:HG23	1:A:-217:GLU:H	1.48	0.77
1:D:-346:ILE:HD13	1:D:-77:PRO:HD3	1.66	0.77
1:D:-346:ILE:HD13	1:D:-77:PRO:CG	2.15	0.77
1:D:-263:PHE:HA	1:D:-260:LYS:CD	2.14	0.76
1:D:-259:LEU:HD12	1:D:-254:TRP:CZ2	2.21	0.76
1:B:-269:ILE:HG22	1:B:-267:PRO:HD3	1.68	0.75
1:B:-226:LEU:HD11	1:B:-213:LEU:HD21	1.69	0.74
1:D:-315:ILE:HD11	1:D:-73:LEU:HD11	1.71	0.72
1:C:-208:LYS:HD2	1:C:-204:LYS:O	1.88	0.72
1:C:-281:PHE:HB3	1:C:-244:ILE:HD13	1.70	0.72
1:D:-346:ILE:HD13	1:D:-77:PRO:CD	2.18	0.72
1:B:24:LYS:HD3	1:B:25:PRO:HD2	1.71	0.72
1:D:-337:ILE:HG13	1:D:-287:PHE:HB2	1.72	0.72
1:B:37:GLU:O	1:B:41:ARG:HG3	1.89	0.72
1:D:-242:TYR:HE2	1:D:-68:LEU:HB3	1.55	0.71
1:D:-27:MET:HA	1:D:-27:MET:HE3	1.72	0.71
1:C:-346:ILE:HD11	1:C:-291:PRO:C	2.15	0.70
1:A:-38:GLU:HA	1:A:-38:GLU:OE2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-220:THR:HG22	1:C:-99:THR:OG1	1.92	0.70
1:D:-315:ILE:CD1	1:D:-73:LEU:HD11	2.22	0.70
1:D:-19:ILE:HD12	1:D:-19:ILE:O	1.90	0.70
1:C:-200:MET:CE	1:C:-126:THR:HB	2.22	0.70
1:A:-153:LEU:CD1	1:A:-144:MET:HE1	2.22	0.69
1:D:-251:VAL:CG2	1:D:-243:ALA:HB3	2.23	0.69
1:D:-220:THR:HG22	1:D:-217:GLU:CD	2.19	0.68
1:C:-280:GLY:HA3	1:C:-16:ASN:O	1.94	0.68
1:C:-200:MET:HE1	1:C:-132:ALA:HB1	1.74	0.68
1:D:-55:VAL:HG11	1:D:-49:LEU:HD21	1.76	0.68
1:B:30:ARG:HD2	1:B:34:ARG:NH2	2.09	0.67
1:D:-343:GLY:O	1:D:-315:ILE:HG23	1.95	0.66
1:D:-170:ILE:HG21	1:D:-13:GLN:NE2	2.10	0.66
1:A:86:THR:OG1	1:B:47:ILE:HA	1.96	0.66
1:D:-291:PRO:O	1:D:-81:ASN:ND2	2.25	0.66
1:A:27:TRP:CD1	1:A:27:TRP:H	2.13	0.65
1:C:-185:ALA:HA	1:C:-92:LYS:HE2	1.78	0.65
1:D:-346:ILE:O	1:D:-346:ILE:HD12	1.97	0.65
1:A:-17:PRO:HA	4:A:401:EDO:H12	1.78	0.65
1:C:-346:ILE:HG22	1:C:-77:PRO:HD2	1.78	0.65
2:F:4:DA:H1'	2:F:5:DT:H5'	1.79	0.64
1:A:-153:LEU:HD12	1:A:-144:MET:HE1	1.79	0.64
1:D:-323:LYS:O	1:D:-320:GLU:HB2	1.98	0.64
1:D:-291:PRO:HG2	1:D:-288:ILE:HG23	1.78	0.64
1:A:24:LYS:HD2	1:A:24:LYS:N	2.12	0.64
1:A:-345:GLU:CG	1:A:-342:LYS:HD3	2.21	0.64
1:B:-153:LEU:CD1	1:B:-144:MET:HE1	2.27	0.64
1:B:-4:ARG:HD2	5:B:404:HOH:O	1.97	0.64
2:E:4:DA:OP2	2:E:4:DA:H2'	1.97	0.64
1:D:-220:THR:HG23	1:D:-217:GLU:H	1.63	0.64
1:A:-259:LEU:HD23	1:A:-241:PRO:HG2	1.79	0.64
1:C:-199:PHE:O	1:C:-197:LEU:HD22	1.98	0.63
1:B:88:ARG:HH11	1:B:88:ARG:CB	2.04	0.63
1:C:-217:GLU:O	1:C:-213:LEU:HD23	1.97	0.63
1:D:88:ARG:HG2	1:D:88:ARG:HH11	1.64	0.63
1:A:47:ILE:O	1:A:51:LEU:HG	1.99	0.63
1:A:82:GLU:HG3	1:A:83:ASP:N	2.13	0.63
1:B:-286:TRP:CD1	1:B:-282:ARG:HG3	2.34	0.62
1:D:-291:PRO:O	1:D:-81:ASN:HB2	1.99	0.62
1:D:-75:LYS:O	1:D:-71:LYS:HG3	1.99	0.62
1:C:75:GLU:OE1	1:D:76:ALA:HB1	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-242:TYR:CD2	1:D:-68:LEU:HB3	2.34	0.62
1:B:-280:GLY:HA3	1:B:-16:ASN:O	2.00	0.62
1:C:-346:ILE:CD1	1:C:-292:GLY:O	2.48	0.62
2:F:5:DT:H2"	2:F:6:DG:OP2	1.99	0.61
1:D:-272:LEU:HD13	1:D:-244:ILE:HG21	1.82	0.61
1:D:-345:GLU:OE1	1:A:27:TRP:HH2	1.84	0.61
1:D:-277:ALA:HB2	1:D:-244:ILE:HG21	1.83	0.61
1:D:-164:ASP:HB2	1:D:17:GLN:HB2	1.83	0.61
1:D:-341:LEU:O	1:D:-313:VAL:HA	2.00	0.61
1:B:23:ARG:HG3	1:B:23:ARG:O	2.01	0.61
1:A:-269:ILE:HD12	1:A:-242:TYR:CE2	2.35	0.60
1:D:42:ALA:O	1:D:46:LYS:HE3	2.00	0.60
1:A:-280:GLY:HA3	1:A:-16:ASN:O	2.01	0.60
1:D:-320:GLU:HG2	1:D:-315:ILE:O	2.01	0.60
1:D:-344:GLU:CG	1:D:-77:PRO:HB2	2.30	0.60
1:C:-259:LEU:HD23	1:C:-241:PRO:HG2	1.82	0.59
1:A:27:TRP:HA	1:A:30:ARG:HG3	1.83	0.59
1:D:-336:ASN:OD1	1:D:-286:TRP:HZ3	1.84	0.59
1:B:-164:ASP:HB3	1:B:17:GLN:NE2	2.18	0.59
1:D:-298:VAL:O	1:D:-295:THR:HG23	2.03	0.59
1:A:-220:THR:HG22	1:A:-217:GLU:CD	2.27	0.59
1:D:74:VAL:HA	1:D:78:TRP:O	2.03	0.59
1:D:-251:VAL:HG21	1:D:-243:ALA:HB3	1.85	0.59
1:D:-115:SER:O	1:D:-111:THR:HG23	2.03	0.58
1:D:-263:PHE:CA	1:D:-260:LYS:HD2	2.21	0.58
1:B:-156:LEU:O	1:B:-152:VAL:HG23	2.02	0.58
1:A:81:GLU:CD	1:A:85:THR:HB	2.28	0.58
1:D:-346:ILE:CD1	1:D:-77:PRO:HD3	2.33	0.58
1:D:-339:ILE:HG12	1:D:-289:ILE:CG1	2.29	0.57
1:B:-191:THR:HG23	5:B:418:HOH:O	2.03	0.57
1:C:-194:PRO:HD3	1:C:-4:ARG:HG3	1.85	0.57
1:A:-301:PHE:CG	1:A:-288:ILE:HD12	2.39	0.57
1:D:-346:ILE:HD12	1:D:-346:ILE:C	2.29	0.57
1:B:71:ALA:O	1:B:74:VAL:HG22	2.04	0.57
1:C:-60:GLU:H	1:C:-60:GLU:CD	2.11	0.57
1:D:-259:LEU:HD11	1:D:-63:LEU:CD1	2.29	0.57
1:C:-219:TRP:O	1:C:-216:ILE:HB	2.05	0.56
1:D:-104:VAL:CG2	1:D:-32:ARG:HG2	2.34	0.56
1:C:-218:GLU:O	1:C:-215:PRO:HD2	2.05	0.56
1:D:-69:PHE:HA	1:D:-65:TYR:HB2	1.87	0.56
1:D:-27:MET:HE3	1:D:-24:ALA:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-55:VAL:HG12	1:D:-49:LEU:HG	1.88	0.56
1:B:88:ARG:HB3	1:B:88:ARG:NH1	2.07	0.56
1:D:-254:TRP:HE3	1:D:-245:LEU:HD23	1.71	0.56
1:D:-258:TYR:CE1	1:D:-43:LYS:HG2	2.40	0.56
1:A:27:TRP:H	1:A:27:TRP:HD1	1.52	0.56
1:D:36:ARG:HD2	5:D:201:HOH:O	2.04	0.55
1:B:-214:ALA:O	1:B:-210:GLU:HG2	2.07	0.55
1:A:88:ARG:NH2	1:B:75:GLU:OE2	2.39	0.55
1:B:-212:ASP:O	1:B:-208:LYS:HG2	2.07	0.55
1:D:-250:ARG:HH11	1:D:-247:GLY:HA2	1.70	0.55
1:B:-17:PRO:HD2	1:B:-12:MET:HE2	1.88	0.55
1:C:-188:LEU:O	1:C:-188:LEU:HD12	2.06	0.54
1:A:-195:GLU:OE1	1:A:-4:ARG:NH2	2.39	0.54
2:F:10:DA:H2''	2:F:11:DA:O5'	2.08	0.54
1:D:-242:TYR:CD2	1:D:-68:LEU:HD23	2.43	0.54
1:A:-286:TRP:CD1	1:A:-282:ARG:HG3	2.42	0.54
1:A:-329:GLY:HA2	1:A:-326:GLU:OE1	2.07	0.54
1:D:-220:THR:HG22	1:D:-217:GLU:OE1	2.07	0.54
1:D:-178:LYS:HD2	1:D:-168:ASP:OD2	2.08	0.54
1:A:31:GLU:O	1:A:35:ARG:HG2	2.07	0.54
1:D:-338:TRP:CE3	1:D:-291:PRO:HG3	2.43	0.54
1:B:-298:VAL:HB	1:B:-293:ASP:HB2	1.90	0.54
2:H:10:DA:H2''	2:H:11:DA:O5'	2.07	0.53
1:C:-200:MET:CE	1:C:-132:ALA:HB1	2.38	0.53
1:D:-272:LEU:HD13	1:D:-244:ILE:CG2	2.37	0.53
1:D:-248:ASN:HD22	1:D:-248:ASN:C	2.10	0.53
1:B:80:VAL:HG22	1:B:86:THR:OG1	2.08	0.53
1:C:-346:ILE:HD12	1:C:-292:GLY:O	2.09	0.53
1:D:-264:ALA:O	1:D:-260:LYS:HE3	2.09	0.53
1:D:-227:LEU:HD21	1:D:-204:LYS:HE3	1.90	0.53
1:D:-269:ILE:CG2	1:D:-242:TYR:HE1	2.22	0.52
1:C:-263:PHE:CE2	1:C:-67:GLU:HG2	2.44	0.52
1:C:-200:MET:HE2	1:C:-126:THR:HB	1.91	0.52
1:D:-278:TYR:HB3	1:D:-272:LEU:HD11	1.92	0.52
1:D:-337:ILE:HG13	1:D:-287:PHE:CB	2.39	0.52
1:D:-247:GLY:C	1:D:-246:LYS:HD2	2.35	0.52
1:A:-300:PRO:HA	1:A:-273:LEU:HD13	1.90	0.52
1:C:-133:ALA:O	1:C:-129:LYS:HG3	2.10	0.52
1:D:-295:THR:O	1:D:-295:THR:OG1	2.25	0.52
2:E:5:DT:H2''	2:E:6:DG:OP2	2.10	0.52
1:D:-254:TRP:CE3	1:D:-245:LEU:HD23	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-4:ARG:NH2	5:B:404:HOH:O	2.42	0.51
1:D:-258:TYR:CZ	1:D:-43:LYS:HG2	2.46	0.51
1:B:41:ARG:HH12	2:F:2:DA:H2'	1.74	0.51
1:D:-269:ILE:HG23	1:D:-242:TYR:HE1	1.76	0.51
1:B:35:ARG:HB3	1:B:35:ARG:CZ	2.40	0.51
1:A:15:ALA:O	1:A:19:ASN:OD1	2.28	0.51
1:D:-320:GLU:CG	1:D:-315:ILE:O	2.59	0.51
1:D:-341:LEU:HB3	1:D:-313:VAL:HG22	1.92	0.50
1:A:-220:THR:HG22	1:A:-217:GLU:CG	2.41	0.50
1:D:-179:PHE:HE2	1:D:-12:MET:HE2	1.76	0.50
1:C:-218:GLU:OE1	1:C:-218:GLU:N	2.43	0.50
1:C:-216:ILE:CD1	1:C:-124:MET:HE1	2.42	0.50
1:D:-344:GLU:HG3	1:D:-77:PRO:CB	2.38	0.50
1:A:-116:TRP:HB2	1:A:-50:PRO:HG2	1.94	0.50
1:B:-152:VAL:HG21	1:B:9:VAL:CG2	2.41	0.50
1:C:-155:THR:HA	1:C:-152:VAL:HG22	1.92	0.50
1:B:-153:LEU:HD11	1:B:-144:MET:HE1	1.92	0.50
1:D:-278:TYR:CB	1:D:-272:LEU:HD11	2.41	0.49
1:D:88:ARG:HG2	1:D:88:ARG:NH1	2.26	0.49
1:D:-220:THR:HG22	1:D:-217:GLU:CG	2.42	0.49
1:D:-15:ILE:HB	1:D:-14:PRO:CD	2.43	0.49
1:B:-194:PRO:HB3	1:B:-5:VAL:HG12	1.93	0.49
1:B:70:LYS:O	1:B:74:VAL:HG13	2.12	0.49
1:C:-305:LEU:C	1:C:-305:LEU:HD12	2.38	0.49
1:D:-269:ILE:HD12	1:D:-242:TYR:CE1	2.47	0.49
1:D:-281:PHE:HE2	1:D:-83:GLY:H	1.61	0.49
1:B:30:ARG:HH11	1:B:34:ARG:HH22	1.59	0.49
1:D:-298:VAL:HG23	1:D:-293:ASP:O	2.13	0.49
1:A:-330:ASN:O	1:A:-326:GLU:HG3	2.12	0.49
1:D:-230:ASN:ND2	1:D:-108:VAL:HG13	2.28	0.48
1:A:-16:ASN:H	4:A:401:EDO:H12	1.78	0.48
1:C:-46:VAL:HG13	1:C:-37:LEU:HD12	1.95	0.48
1:D:-340:VAL:HG12	1:D:-312:THR:OG1	2.13	0.48
1:D:-153:LEU:CD1	1:D:-144:MET:HE1	2.43	0.48
1:D:-131:PHE:HA	1:D:-126:THR:HG22	1.93	0.48
1:A:30:ARG:HH22	2:E:5:DT:H3'	1.78	0.48
1:C:61:LYS:HG2	1:C:62:HIS:CD2	2.49	0.48
1:D:-89:VAL:HG23	1:D:-20:GLU:O	2.14	0.48
1:D:-276:GLN:HB2	1:D:-249:TYR:HE2	1.78	0.48
1:D:-250:ARG:NH2	1:D:-245:LEU:HD11	2.29	0.48
1:D:-241:PRO:O	1:D:-240:ILE:HD12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-227:LEU:CD2	1:D:-204:LYS:HG3	2.44	0.48
1:D:-194:PRO:HB3	1:D:-5:VAL:HG12	1.94	0.48
1:C:-102:VAL:HG12	1:C:-101:LEU:O	2.13	0.48
1:D:-251:VAL:HG13	1:D:-251:VAL:O	2.13	0.48
1:D:-275:SER:O	1:D:-273:LEU:HD12	2.14	0.48
2:F:-3:DT:H2''	2:F:-2:DT:H5'	1.96	0.48
1:D:-104:VAL:HG21	1:D:-32:ARG:HG2	1.95	0.47
1:A:-212:ASP:HA	1:A:-202:ALA:HB2	1.96	0.47
1:A:-184:ASP:HA	1:A:-95:GLN:OE1	2.14	0.47
1:B:48:TYR:HA	1:B:51:LEU:HD12	1.95	0.47
1:A:-346:ILE:HG21	1:A:-290:ASP:OD1	2.14	0.47
1:D:-94:PRO:HB3	1:D:-22:LYS:HD3	1.95	0.47
1:C:-226:LEU:HD21	1:C:-222:PRO:HD3	1.95	0.47
1:D:-297:ALA:HB3	1:D:-273:LEU:HD23	1.96	0.47
1:C:72:LEU:HD12	1:C:72:LEU:O	2.15	0.47
1:A:-180:ALA:O	1:A:-167:VAL:HA	2.14	0.47
1:C:-263:PHE:CZ	1:C:-67:GLU:HG2	2.49	0.47
1:A:81:GLU:CG	1:A:85:THR:HB	2.45	0.47
1:D:-269:ILE:HB	1:D:-245:LEU:O	2.15	0.47
1:D:-64:LEU:C	1:D:-62:THR:H	2.23	0.47
1:D:-41:TYR:CE2	1:D:-37:LEU:HD11	2.50	0.47
2:F:6:DG:H2'	2:F:7:DT:H72	1.96	0.47
1:C:60:PRO:HG2	1:C:63:CYS:HB3	1.98	0.46
1:A:-345:GLU:HG3	1:A:-342:LYS:CD	2.25	0.46
1:A:27:TRP:CD1	1:A:27:TRP:N	2.82	0.46
1:D:-254:TRP:CE3	1:D:-245:LEU:CD2	2.99	0.46
1:B:-208:LYS:HA	1:B:-208:LYS:HD3	1.67	0.46
1:B:-17:PRO:HD2	1:B:-12:MET:CE	2.45	0.46
1:B:-259:LEU:HD23	1:B:-241:PRO:HG2	1.96	0.46
1:B:-194:PRO:CB	1:B:-5:VAL:HG12	2.46	0.46
1:D:-40:GLU:HA	1:D:-40:GLU:OE1	2.15	0.46
1:A:85:THR:OG1	1:B:46:LYS:NZ	2.40	0.46
1:D:-300:PRO:HA	1:D:-273:LEU:CD2	2.46	0.46
1:D:-269:ILE:HG23	1:D:-242:TYR:CE1	2.51	0.46
1:B:-339:ILE:HG12	1:B:-289:ILE:HB	1.96	0.46
1:C:-130:ASN:H	1:C:-130:ASN:HD22	1.63	0.46
1:D:-243:ALA:HB1	1:D:-84:ALA:C	2.41	0.45
1:B:-259:LEU:HD22	1:B:-254:TRP:CZ2	2.51	0.45
1:D:-74:GLU:HA	1:D:-71:LYS:HB2	1.97	0.45
1:A:-342:LYS:HG3	5:A:528:HOH:O	2.16	0.45
1:A:35:ARG:HB3	1:A:38:ARG:HH12	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-304:GLU:HB2	1:C:-282:ARG:HD2	1.97	0.45
1:D:-269:ILE:CG2	1:D:-242:TYR:CE1	2.98	0.45
1:A:-219:TRP:CD1	1:A:-100:PRO:HB2	2.51	0.45
1:A:-189:PRO:HG3	1:A:-91:PRO:HA	1.97	0.45
1:B:-337:ILE:O	1:B:-309:HIS:HA	2.16	0.45
1:B:60:PRO:O	1:B:63:CYS:HB3	2.16	0.45
1:A:57:TYR:OH	1:A:75:GLU:OE1	2.26	0.45
1:D:-249:TYR:CB	1:D:-244:ILE:CD1	2.92	0.45
2:H:-3:DT:H2''	2:H:-2:DT:H5'	1.99	0.45
1:D:-12:MET:HE2	1:D:-12:MET:HA	1.98	0.45
1:D:-315:ILE:HD12	1:D:-73:LEU:CD2	2.38	0.45
1:A:30:ARG:NH2	2:E:5:DT:H3'	2.31	0.45
1:D:-153:LEU:HD11	1:D:-144:MET:HE1	1.98	0.45
1:B:-260:LYS:C	1:B:-259:LEU:HD12	2.42	0.45
1:A:-145:HIS:O	1:A:-144:MET:HG3	2.17	0.45
1:D:-243:ALA:HB1	1:D:-84:ALA:H	1.82	0.44
2:G:0:DA:H2''	2:G:1:DC:C5	2.51	0.44
1:B:-211:LYS:HE2	1:B:-211:LYS:HB2	1.79	0.44
1:A:-346:ILE:H	1:A:-346:ILE:HG13	1.50	0.44
1:B:-38:GLU:HG3	5:B:441:HOH:O	2.17	0.44
1:B:31:GLU:O	1:B:35:ARG:HG3	2.17	0.44
1:C:-124:MET:HE3	1:C:-124:MET:HB2	1.82	0.44
2:F:4:DA:C1'	2:F:5:DT:H5'	2.47	0.44
1:C:51:LEU:HD21	1:C:72:LEU:HD22	2.00	0.44
1:C:-190:TRP:N	1:C:-189:PRO:CD	2.81	0.44
1:C:-300:PRO:HA	1:C:-273:LEU:HD13	2.00	0.44
1:C:-287:PHE:HA	1:C:-85:SER:O	2.17	0.44
1:D:-2:ALA:HB2	1:D:16:ALA:HB2	1.99	0.44
1:B:-119:PRO:HA	1:B:-116:TRP:CE2	2.53	0.43
1:B:-115:SER:HB3	5:B:428:HOH:O	2.17	0.43
1:D:-288:ILE:O	1:D:-288:ILE:HG13	2.17	0.43
1:A:-213:LEU:O	1:A:-213:LEU:HD12	2.19	0.43
1:A:-119:PRO:HA	1:A:-116:TRP:CE2	2.53	0.43
1:A:85:THR:HA	1:B:46:LYS:HG2	2.00	0.43
1:B:-61:ASP:OD1	1:B:-42:SER:OG	2.36	0.43
1:C:-333:LYS:HD2	5:C:626:HOH:O	2.18	0.43
1:D:-320:GLU:O	1:D:-316:GLY:N	2.42	0.43
1:D:-179:PHE:HE2	1:D:-12:MET:CE	2.31	0.43
1:A:-337:ILE:O	1:A:-309:HIS:HA	2.18	0.43
1:B:-128:GLY:HA2	5:B:421:HOH:O	2.17	0.43
1:D:-179:PHE:CE2	1:D:-12:MET:CE	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLU:OE2	1:A:70:LYS:HE3	2.19	0.43
1:B:-190:TRP:HA	1:B:-187:ILE:HD12	2.01	0.43
2:F:4:DA:H2''	2:F:5:DT:O5'	2.17	0.43
1:C:61:LYS:HE3	1:C:62:HIS:NE2	2.34	0.43
1:D:-193:TYR:HB2	3:M:2:GLC:O5	2.19	0.43
1:D:-95:GLN:HB3	1:D:-92:LYS:NZ	2.33	0.43
1:A:80:VAL:CG1	1:A:86:THR:HG23	2.40	0.43
1:C:-155:THR:O	1:C:-152:VAL:HG22	2.18	0.43
1:D:-101:LEU:HB2	1:D:-93:SER:HB2	2.00	0.43
1:A:-226:LEU:HD22	1:A:-125:ALA:HB1	2.00	0.42
1:A:82:GLU:HG3	1:A:83:ASP:H	1.80	0.42
1:A:-220:THR:HG23	1:A:-217:GLU:N	2.23	0.42
1:B:-53:LYS:HE3	1:B:-53:LYS:N	2.34	0.42
1:B:78:TRP:CE3	1:B:86:THR:HG22	2.54	0.42
1:C:-251:VAL:HG21	1:C:-241:PRO:HD3	2.01	0.42
1:C:-216:ILE:HD13	1:C:-216:ILE:HA	1.92	0.42
1:D:-315:ILE:HG21	1:D:-73:LEU:HD21	2.02	0.42
1:C:19:ASN:OD1	1:C:22:ARG:NH1	2.53	0.42
1:D:-300:PRO:HA	1:D:-273:LEU:HD21	2.00	0.42
1:D:-167:VAL:HG13	1:D:17:GLN:OE1	2.18	0.42
1:A:52:ARG:NH2	1:A:63:CYS:O	2.43	0.42
1:D:-291:PRO:HG2	1:D:-288:ILE:CG2	2.45	0.42
1:D:38:ARG:HG2	1:D:38:ARG:HH11	1.85	0.42
1:C:-40:GLU:OE1	1:C:-40:GLU:HA	2.19	0.42
1:A:-94:PRO:HD2	1:A:-92:LYS:NZ	2.34	0.42
1:A:34:ARG:CG	2:E:4:DA:H2'	2.50	0.42
1:D:-270:GLU:HG3	1:D:-246:LYS:HB3	2.02	0.42
1:D:-104:VAL:HG23	1:D:-32:ARG:HG2	2.01	0.42
1:D:-81:ASN:HB3	1:D:-78:SER:HB2	2.02	0.42
1:A:-172:TYR:HE2	4:A:401:EDO:H11	1.83	0.42
1:B:-8:TRP:CD1	3:K:2:GLC:H4	2.55	0.42
1:A:-153:LEU:O	1:A:-150:LEU:HB2	2.20	0.42
1:B:30:ARG:CD	1:B:34:ARG:HH12	2.32	0.42
1:D:-55:VAL:CG1	1:D:-49:LEU:HD21	2.48	0.42
1:A:-98:PHE:CE2	1:A:-97:LYS:HD2	2.55	0.42
2:E:3:DT:H2''	2:E:4:DA:C8	2.55	0.42
1:C:-200:MET:HB2	1:C:-200:MET:HE3	1.82	0.41
1:C:57:TYR:O	1:C:58:ASN:HB2	2.20	0.41
1:D:-318:ASP:OD2	1:D:-65:TYR:OH	2.34	0.41
2:F:2:DA:H1'	2:F:3:DT:H5'	2.01	0.41
1:C:-210:GLU:H	1:C:-210:GLU:HG3	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-27:MET:HA	1:D:-27:MET:CE	2.41	0.41
1:A:-153:LEU:HD12	1:A:-144:MET:CE	2.48	0.41
1:A:-17:PRO:HD2	1:A:-12:MET:HE2	2.02	0.41
1:A:-184:ASP:OD1	1:A:-95:GLN:OE1	2.39	0.41
1:C:1:ASN:HB3	1:C:7:GLN:HB2	2.02	0.41
1:D:-259:LEU:HB2	1:D:-254:TRP:NE1	2.36	0.41
1:A:-94:PRO:HD2	1:A:-92:LYS:HZ1	1.85	0.41
1:C:-119:PRO:HA	1:C:-116:TRP:CE2	2.56	0.41
1:D:-259:LEU:CD2	1:D:-44:LEU:HA	2.51	0.41
1:D:-230:ASN:ND2	1:D:-227:LEU:HD12	2.36	0.41
1:A:24:LYS:N	1:A:24:LYS:CD	2.83	0.41
1:D:-69:PHE:O	1:D:-65:TYR:HB2	2.21	0.41
1:C:-244:ILE:C	1:C:-244:ILE:HD12	2.46	0.40
1:D:-216:ILE:N	1:D:-215:PRO:CD	2.84	0.40
1:A:-301:PHE:N	1:A:-300:PRO:HD2	2.36	0.40
1:A:-92:LYS:HG2	1:A:-22:LYS:O	2.21	0.40
1:B:-287:PHE:HA	1:B:-85:SER:O	2.21	0.40
1:B:-226:LEU:HA	1:B:-226:LEU:HD23	1.84	0.40
1:C:-317:THR:HG21	1:C:-70:GLU:OE2	2.22	0.40
1:B:30:ARG:HD3	1:B:34:ARG:HH12	1.86	0.40
1:B:-231:TYR:CE2	1:B:-223:PRO:HD3	2.56	0.40
1:D:-269:ILE:HD12	1:D:-242:TYR:CZ	2.57	0.40
1:D:-226:LEU:HD11	1:D:-213:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/453 (96%)	429 (99%)	6 (1%)	0	100	100
1	B	434/453 (96%)	430 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	434/453 (96%)	426 (98%)	8 (2%)	0	100	100
1	D	434/453 (96%)	422 (97%)	12 (3%)	0	100	100
All	All	1737/1812 (96%)	1707 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	344/356 (97%)	325 (94%)	19 (6%)	18	25
1	B	343/356 (96%)	336 (98%)	7 (2%)	50	67
1	C	343/356 (96%)	335 (98%)	8 (2%)	45	62
1	D	343/356 (96%)	329 (96%)	14 (4%)	26	38
All	All	1373/1424 (96%)	1325 (96%)	48 (4%)	31	44

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	-295	THR
1	C	-216	ILE
1	C	-208	LYS
1	C	-197	LEU
1	C	-146	LYS
1	C	-90	PHE
1	C	-63	LEU
1	C	-60	GLU
1	D	-345	GLU
1	D	-315	ILE
1	D	-295	THR
1	D	-289	ILE
1	D	-210	GLU
1	D	-126	THR

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Mol	Chain	Res	Type
1	D	-111	THR
1	D	-103	THR
1	D	-90	PHE
1	D	-82	ILE
1	D	-68	LEU
1	D	-19	ILE
1	D	23	ARG
1	D	56	ASP
1	A	-348	MET
1	A	-346	ILE
1	A	-345	GLU
1	A	-305	LEU
1	A	-288	ILE
1	A	-275	SER
1	A	-210	GLU
1	A	-146	LYS
1	A	-144	MET
1	A	-124	MET
1	A	-90	PHE
1	A	-11	SER
1	A	22	ARG
1	A	29	GLU
1	A	47	ILE
1	A	69	LEU
1	A	79	VAL
1	A	82	GLU
1	A	88	ARG
1	B	-346	ILE
1	B	-226	LEU
1	B	-178	LYS
1	B	-144	MET
1	B	-53	LYS
1	B	0	ILE
1	B	88	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	-230	ASN
1	C	-143	ASN
1	C	-130	ASN
1	D	-230	ASN

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Mol	Chain	Res	Type
1	D	-147	ASN
1	A	-143	ASN
1	A	7	GLN
1	A	19	ASN
1	B	-276	GLN
1	B	17	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 ⓘ

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GLC	J	1	3	12,12,12	0.50	0	17,17,17	0.72	0
3	GLC	J	2	3	11,11,12	0.67	0	15,15,17	1.01	0
3	GLC	K	1	3	12,12,12	0.51	0	17,17,17	0.96	0
3	GLC	K	2	3	11,11,12	0.72	0	15,15,17	1.01	0
3	GLC	L	1	3	12,12,12	0.45	0	17,17,17	0.85	0
3	GLC	L	2	3	11,11,12	0.54	0	15,15,17	1.09	2 (13%)
3	GLC	M	1	3	12,12,12	0.54	0	17,17,17	0.64	0
3	GLC	M	2	3	11,11,12	0.62	0	15,15,17	0.91	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	J	1	3	-	0/2/22/22	0/1/1/1
3	GLC	J	2	3	-	0/2/19/22	0/1/1/1
3	GLC	K	1	3	-	0/2/22/22	0/1/1/1
3	GLC	K	2	3	-	0/2/19/22	0/1/1/1
3	GLC	L	1	3	-	0/2/22/22	0/1/1/1
3	GLC	L	2	3	-	0/2/19/22	0/1/1/1
3	GLC	M	1	3	-	0/2/22/22	0/1/1/1
3	GLC	M	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	2	GLC	O5-C5-C6	2.20	110.66	107.20
3	L	2	GLC	C2-C3-C4	-2.13	107.20	110.89

There are no chirality outliers.

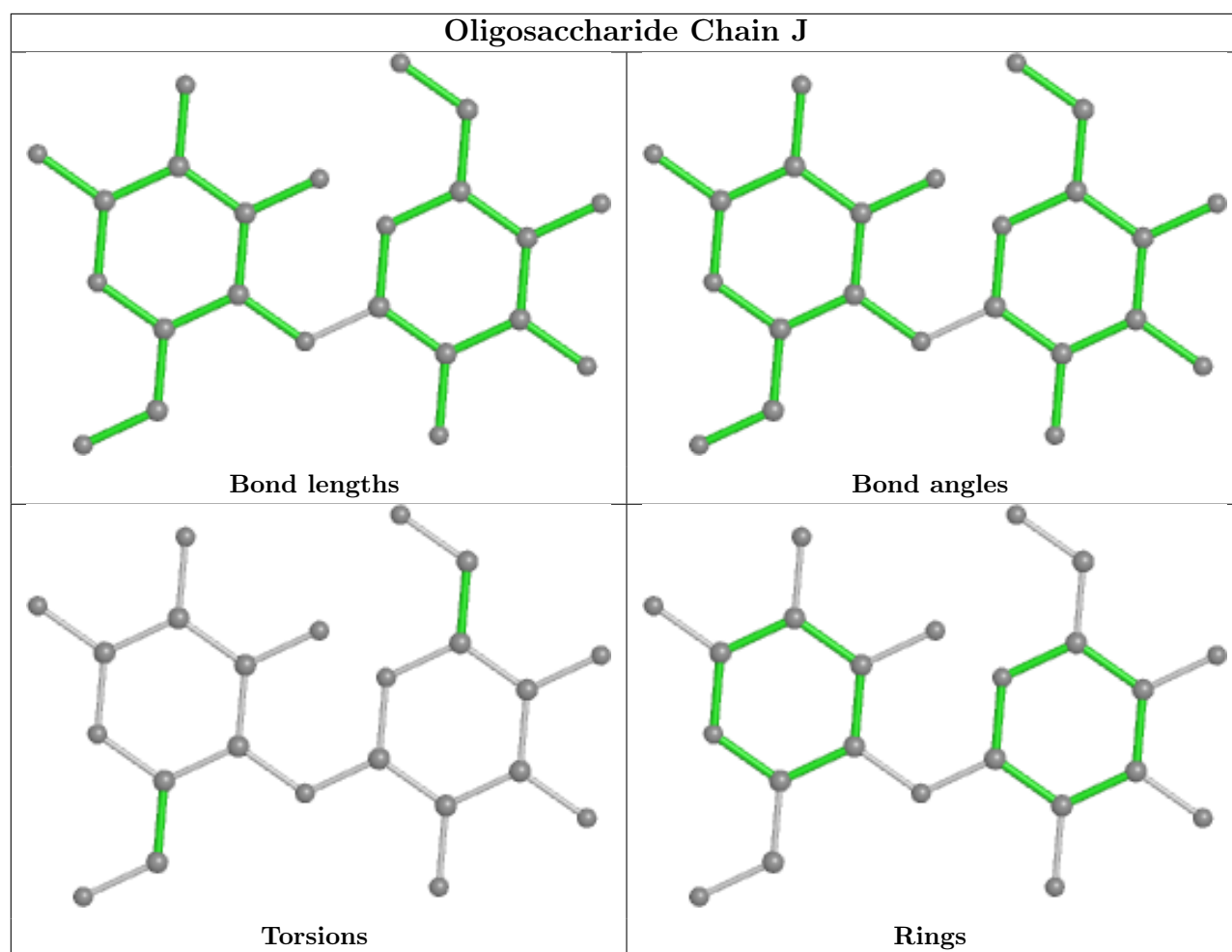
There are no torsion outliers.

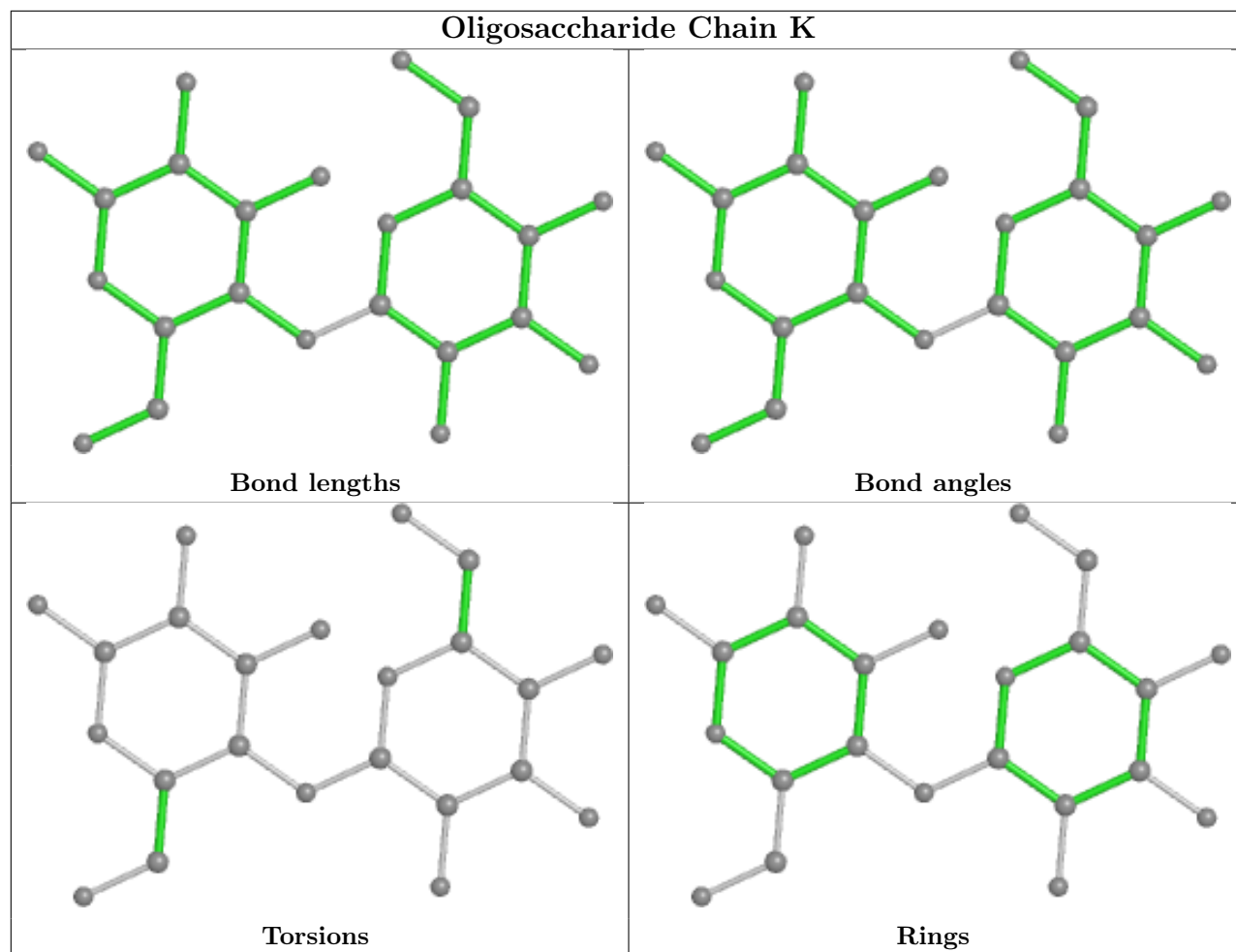
There are no ring outliers.

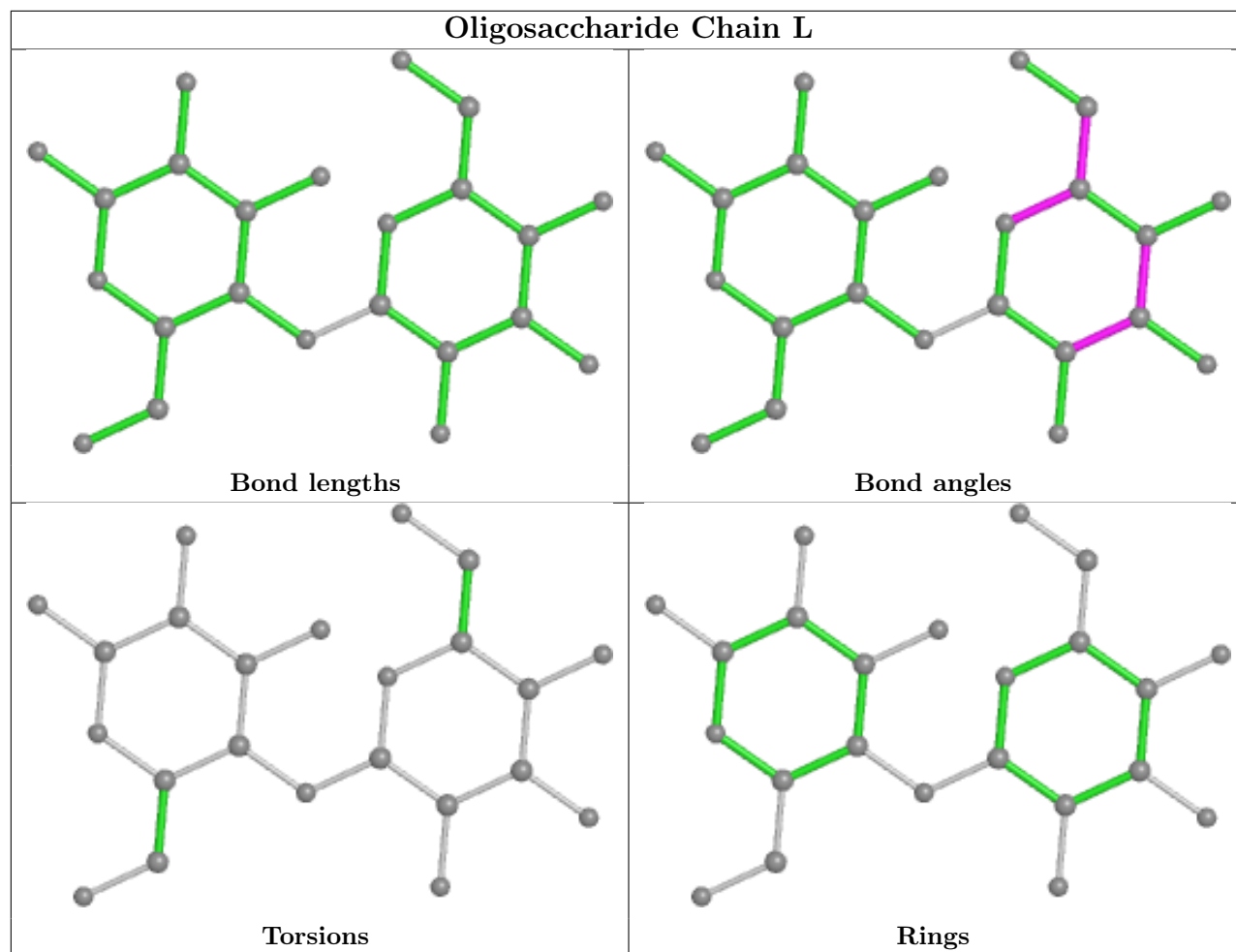
2 monomers are involved in 2 short contacts:

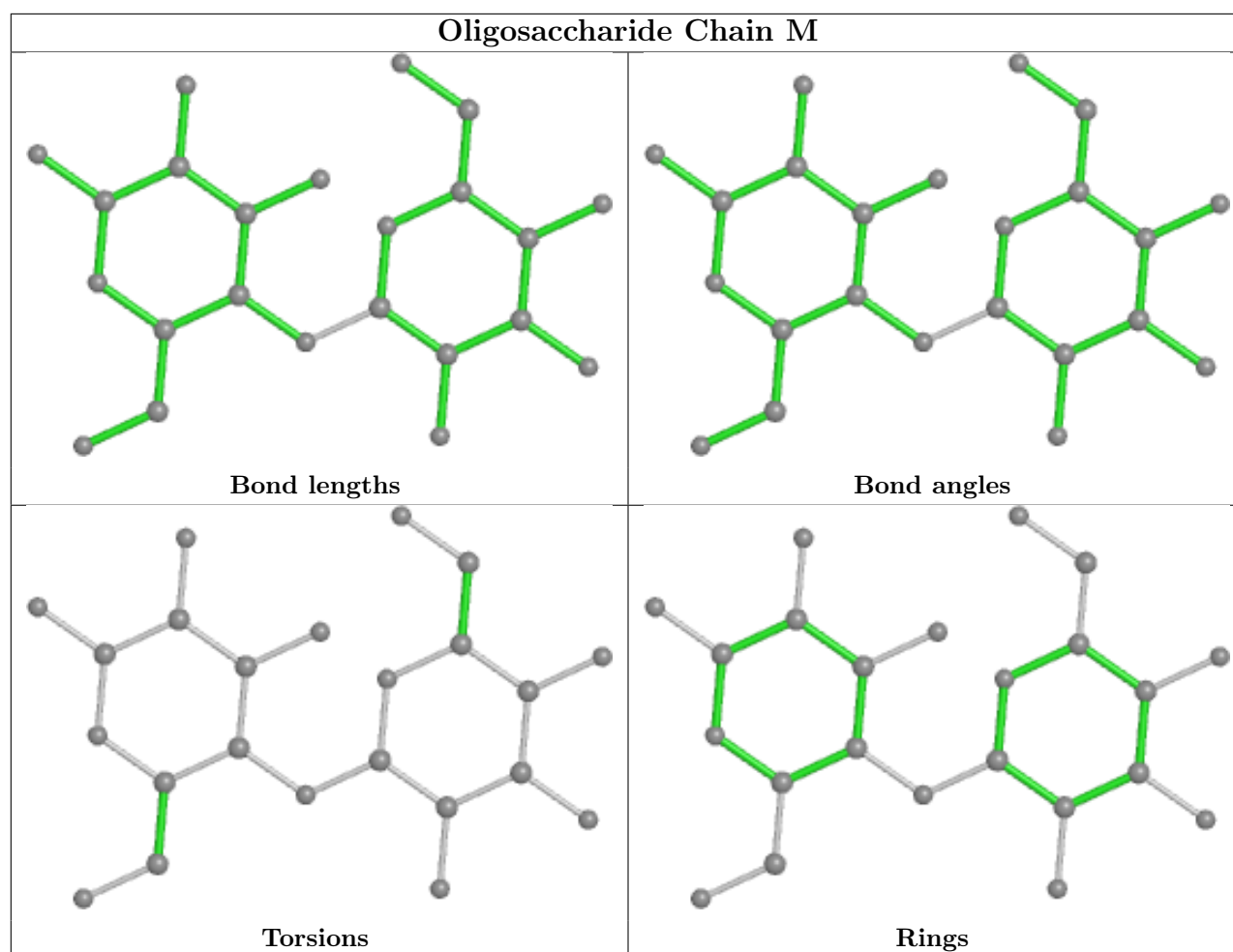
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	2	GLC	1	0
3	K	2	GLC	1	0

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









5.6 Ligand geometry [i](#)

5 ligands 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	$\# Z > 2$
4	EDO	B	302	-	3,3,3	0.52	0	2,2,2	0.32	0
4	EDO	C	501	-	3,3,3	0.50	0	2,2,2	0.31	0
4	EDO	B	303	-	3,3,3	0.46	0	2,2,2	0.46	0
4	EDO	B	301	-	3,3,3	0.48	0	2,2,2	0.80	0
4	EDO	A	401	-	3,3,3	0.48	0	2,2,2	0.40	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	302	-	-	0/1/1/1	-
4	EDO	C	501	-	-	0/1/1/1	-
4	EDO	B	303	-	-	0/1/1/1	-
4	EDO	B	301	-	-	1/1/1/1	-
4	EDO	A	401	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	EDO	O1-C1-C2-O2
4	A	401	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	EDO	3	0

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(Å ²)	Q<0.9
1	A	437/453 (96%)	0.13	10 (2%) 61 62	27, 51, 90, 129	0
1	B	436/453 (96%)	-0.01	8 (1%) 67 69	27, 44, 86, 97	0
1	C	436/453 (96%)	0.11	7 (1%) 70 71	30, 56, 91, 129	0
1	D	436/453 (96%)	0.55	33 (7%) 21 24	34, 66, 110, 129	0
2	E	15/15 (100%)	0.04	0 100 100	63, 75, 109, 114	0
2	F	15/15 (100%)	0.38	0 100 100	55, 90, 108, 113	0
2	G	15/15 (100%)	-0.49	0 100 100	43, 47, 69, 74	0
2	H	15/15 (100%)	-0.58	0 100 100	43, 52, 58, 60	0
All	All	1805/1872 (96%)	0.18	58 (3%) 50 53	27, 55, 97, 129	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-109	ALA	4.3
1	A	27	TRP	3.9
1	D	-271	ALA	3.9
1	D	-311	VAL	3.6
1	D	-288	ILE	3.6
1	D	-277	ALA	3.5
1	D	-287	PHE	3.4
1	D	-266	ALA	3.2
1	D	-341	LEU	3.2
1	D	-73	LEU	3.2
1	C	-207	ALA	3.1
1	A	-7	TYR	3.1
1	D	-313	VAL	3.0
1	A	26	SER	3.0
1	D	-343	GLY	3.0
1	D	-68	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	-346	ILE	2.9
1	D	-314	LYS	2.9
1	D	-82	ILE	2.9
1	A	28	ARG	2.9
1	D	-312	THR	2.9
1	D	-244	ILE	2.7
1	D	-79	ALA	2.7
1	C	-346	ILE	2.7
1	D	-80	ALA	2.7
1	B	-7	TYR	2.6
1	D	-339	ILE	2.6
1	D	-7	TYR	2.5
1	D	26	SER	2.5
1	D	-269	ILE	2.5
1	D	-297	ALA	2.5
1	C	-213	LEU	2.4
1	C	-7	TYR	2.4
1	D	-176	ALA	2.4
1	D	-325	VAL	2.4
1	D	-249	TYR	2.3
1	D	-289	ILE	2.3
1	B	59	LEU	2.3
1	B	42	ALA	2.3
1	C	-111	THR	2.3
1	B	-294	GLY	2.3
1	A	42	ALA	2.2
1	B	60	PRO	2.2
1	B	62	HIS	2.2
1	B	27	TRP	2.2
1	A	32	ASN	2.2
1	A	34	ARG	2.2
1	C	-319	LYS	2.2
1	D	-242	TYR	2.2
1	D	-72	ALA	2.2
1	A	-346	ILE	2.2
1	A	-143	ASN	2.2
1	D	-329	GLY	2.1
1	D	-340	VAL	2.1
1	D	-315	ILE	2.1
1	B	-205	GLY	2.0
1	D	-337	ILE	2.0
1	A	-226	LEU	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 ⓘ

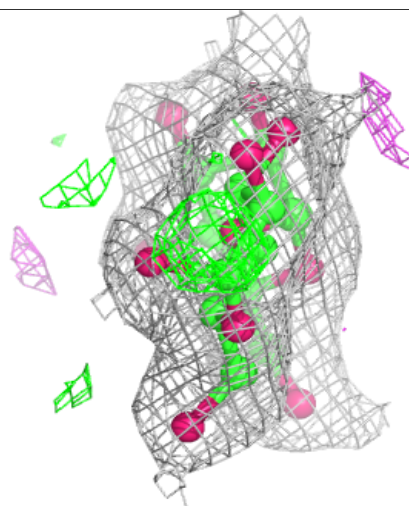
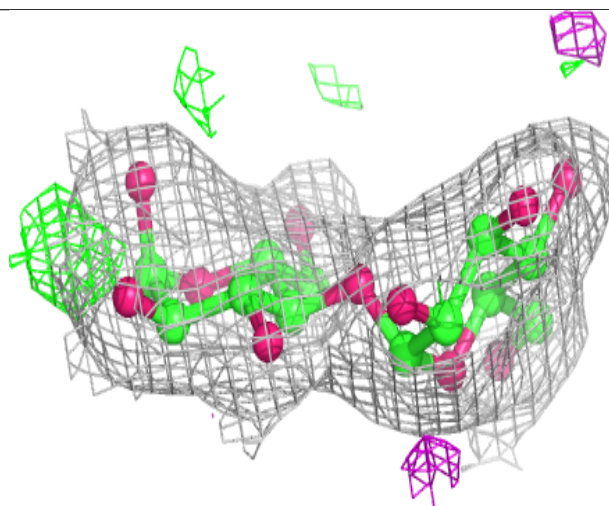
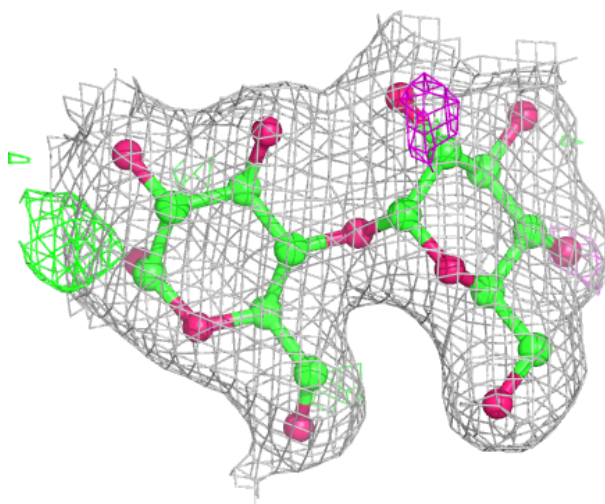
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	L	2	11/12	0.92	0.09	30,36,38,39	0
3	GLC	J	2	11/12	0.95	0.08	34,37,38,39	0
3	GLC	K	1	12/12	0.95	0.06	30,34,38,39	0
3	GLC	L	1	12/12	0.95	0.08	29,37,40,41	0
3	GLC	J	1	12/12	0.95	0.07	31,36,40,44	0
3	GLC	K	2	11/12	0.97	0.05	29,31,34,35	0
3	GLC	M	1	12/12	-	-	44,50,54,58	0
3	GLC	M	2	11/12	-	-	44,48,55,58	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.

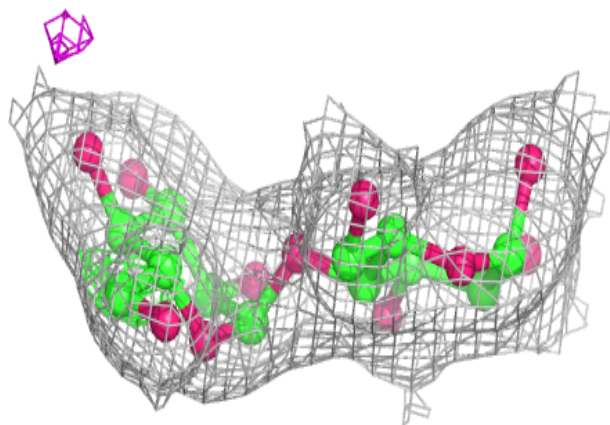
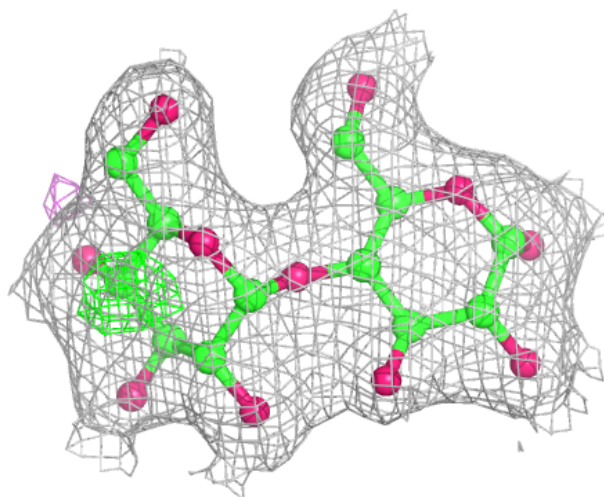
Electron density around Chain J:

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



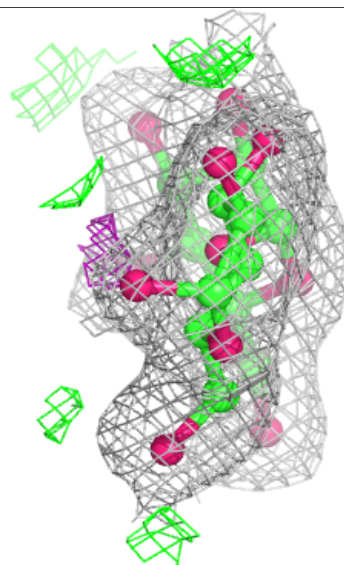
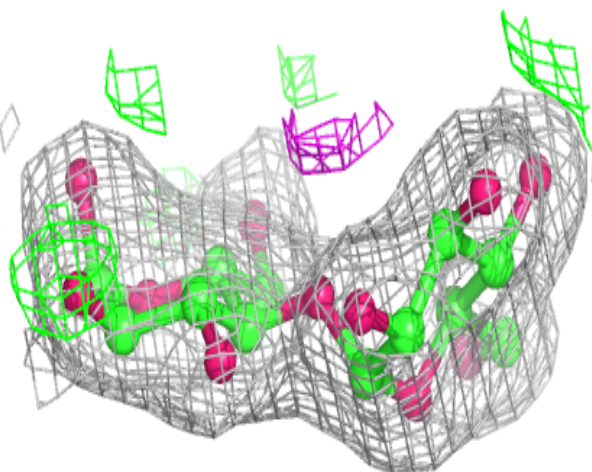
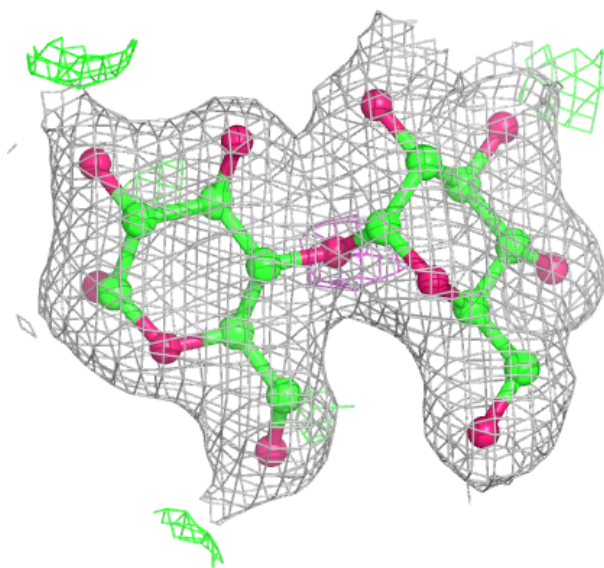
Electron density around Chain K:

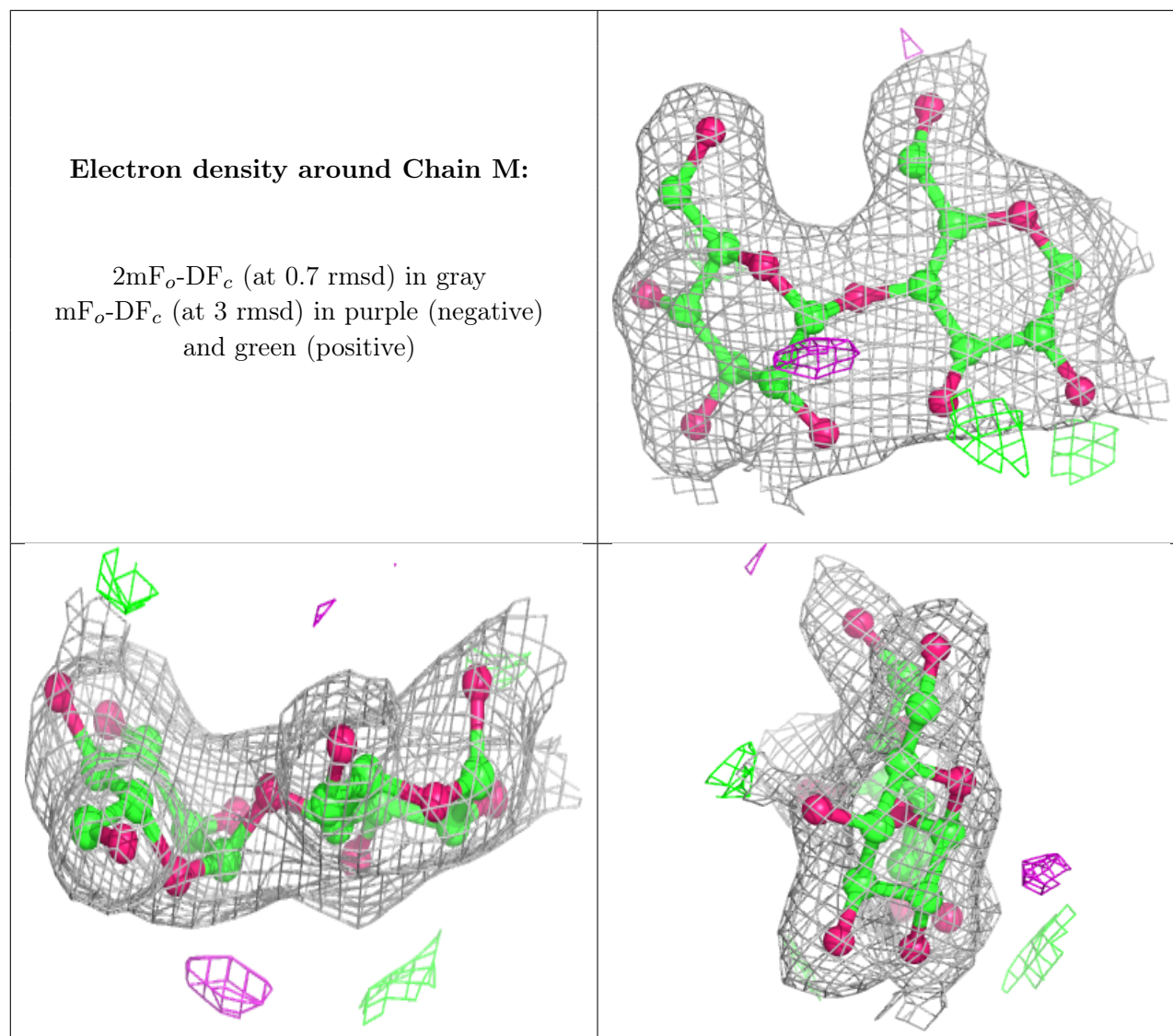
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	EDO	A	401	4/4	0.89	0.13	46,59,71,71	0
4	EDO	B	301	4/4	0.92	0.11	53,64,73,73	0
4	EDO	B	303	4/4	0.93	0.11	46,56,59,62	0
4	EDO	C	501	4/4	0.94	0.09	42,51,60,60	0
4	EDO	B	302	4/4	0.95	0.14	35,43,45,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.