



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:35 PM UTC

PDB ID : 6SWR / pdb_00006swr
Title : Crystal structure of the lysosomal potassium channel MtTMEM175 T38A mutant soaked with zinc
Authors : Brunner, J.D.; Jakob, R.P.; Schulze, T.; Neldner, Y.; Moroni, A.; Thiel, G.; Maier, T.; Schenck, S.
Deposited on : 2019-09-23
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 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:

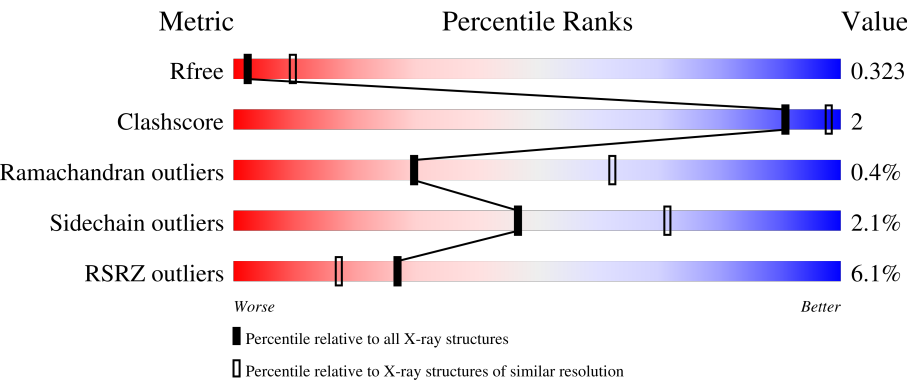
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 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	486	6% 92% 5%
1	D	486	5% 92% 5%
2	B	255	9% 79% 10% 10%
2	E	255	4% 77% 8% 13%

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Mol	Chain	Length	Quality of chain
3	C	2	 100%
3	F	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	K	B	502	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21866 atoms, of which 10922 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 Nanobody, Maltose/maltodextrin-binding periplasmic protein, Maltodextrin-binding protein, Maltose/maltodextrin-binding periplasmic protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	460	Total	C	H	N	O	S	0	0	0
			7080	2283	3517	592	678	10			
1	D	460	Total	C	H	N	O	S	0	0	0
			7080	2283	3517	592	678	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	484	PRO	ARG	conflict	UNP P0AEX9
A	485	GLY	ILE	conflict	UNP P0AEX9
A	486	ALA	THR	conflict	UNP P0AEX9
D	484	PRO	ARG	conflict	UNP P0AEX9
D	485	GLY	ILE	conflict	UNP P0AEX9
D	486	ALA	THR	conflict	UNP P0AEX9

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	230	Total	C	H	N	O	S	0	0	0
			3794	1265	1923	283	315	8			
2	E	222	Total	C	H	N	O	S	0	0	0
			3664	1224	1855	272	305	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP E4TN31
B	1	SER	-	expression tag	UNP E4TN31
B	38	ALA	THR	conflict	UNP E4TN31
B	248	ALA	-	expression tag	UNP E4TN31
B	249	LEU	-	expression tag	UNP E4TN31

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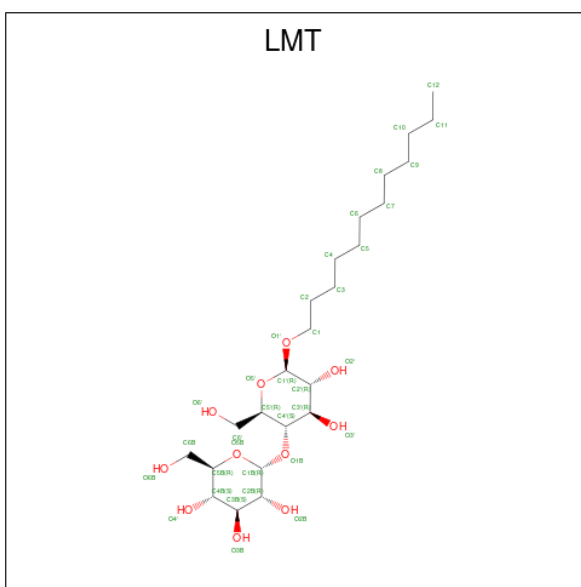
Chain	Residue	Modelled	Actual	Comment	Reference
B	250	GLU	-	expression tag	UNP E4TN31
B	251	VAL	-	expression tag	UNP E4TN31
B	252	LEU	-	expression tag	UNP E4TN31
B	253	PHE	-	expression tag	UNP E4TN31
B	254	GLN	-	expression tag	UNP E4TN31
E	0	MET	-	initiating methionine	UNP E4TN31
E	1	SER	-	expression tag	UNP E4TN31
E	38	ALA	THR	conflict	UNP E4TN31
E	248	ALA	-	expression tag	UNP E4TN31
E	249	LEU	-	expression tag	UNP E4TN31
E	250	GLU	-	expression tag	UNP E4TN31
E	251	VAL	-	expression tag	UNP E4TN31
E	252	LEU	-	expression tag	UNP E4TN31
E	253	PHE	-	expression tag	UNP E4TN31
E	254	GLN	-	expression tag	UNP E4TN31

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	H	O	0	0	0
			45	12	22	11			
3	F	2	Total	C	H	O	0	0	0
			45	12	22	11			

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 63	C 19	H 33	O 11	0	0
4	E	1	Total 63	C 19	H 33	O 11	0	0

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0

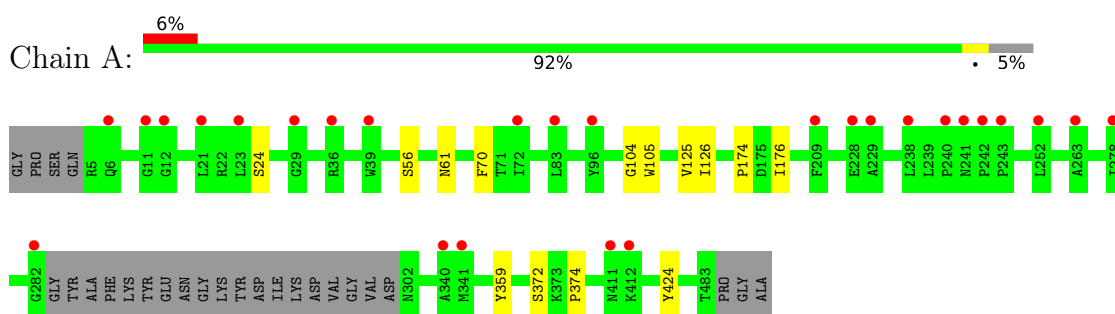
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total O 3 3	0	0
6	B	8	Total O 8 8	0	0
6	D	13	Total O 13 13	0	0
6	E	7	Total O 7 7	0	0

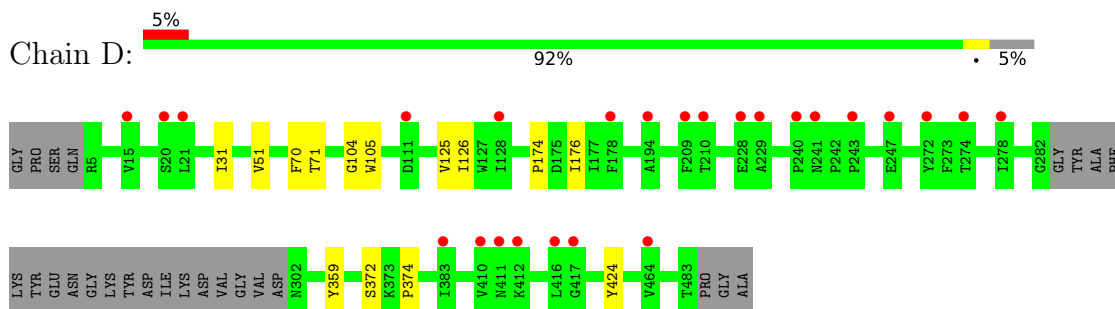
3 Residue-property plots [i](#)

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

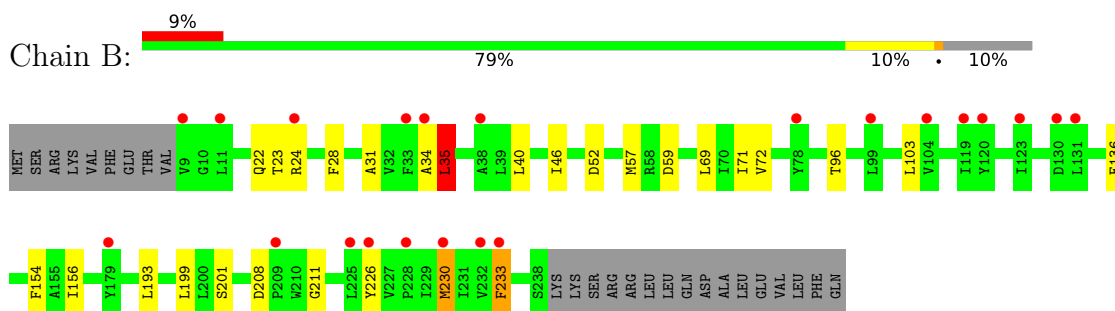
- Molecule 1: Nanobody, Maltose/maltodextrin-binding periplasmic protein, Maltodextrin-binding protein, Maltose/maltodextrin-binding periplasmic protein



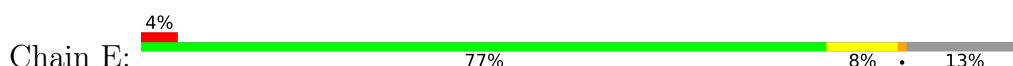
- Molecule 1: Nanobody, Maltose/maltodextrin-binding periplasmic protein, Maltodextrin-binding protein, Maltose/maltodextrin-binding periplasmic protein

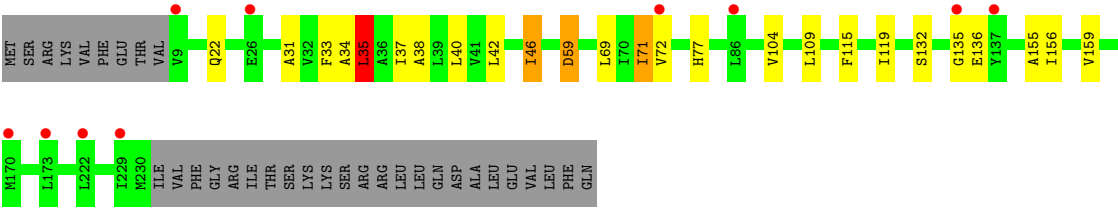


- Molecule 2: Uncharacterized protein



- Molecule 2: Uncharacterized protein





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

Chain C: 100%



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

Chain F: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	129.79Å 131.61Å 151.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 3.20 49.72 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.72-3.20) 99.5 (49.72-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 3.17Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.269 , 0.299 0.297 , 0.323	Depositor DCC
R_{free} test set	2132 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	100.4	Xtriage
Anisotropy	0.862	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 183.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	21866	wwPDB-VP
Average B, all atoms (Å ²)	224.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.65	0/3649	1.27	7/4956 (0.1%)
1	D	0.63	0/3649	1.14	4/4956 (0.1%)
2	B	1.07	6/1921 (0.3%)	1.42	10/2612 (0.4%)
2	E	1.05	6/1858 (0.3%)	1.26	7/2527 (0.3%)
All	All	0.81	12/11077 (0.1%)	1.26	28/15051 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	35	LEU	CB-CG	19.82	1.93	1.53
2	E	35	LEU	CB-CG	19.69	1.92	1.53
2	E	34	ALA	C-N	15.07	1.53	1.33
2	B	34	ALA	C-N	12.51	1.50	1.33
2	B	35	LEU	CA-C	-10.21	1.39	1.52
2	E	35	LEU	CA-C	-8.94	1.41	1.52
2	B	156	ILE	CG1-CD1	-6.49	1.26	1.51
2	B	35	LEU	N-CA	-6.46	1.38	1.46
2	E	35	LEU	CG-CD2	-5.58	1.34	1.52
2	E	35	LEU	C-N	5.52	1.40	1.33
2	B	35	LEU	C-N	5.47	1.40	1.33
2	E	35	LEU	N-CA	-5.43	1.39	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	GLY	N-CA-C	12.11	127.14	112.49
2	B	233	PHE	CA-CB-CG	-9.71	104.09	113.80
1	D	104	GLY	N-CA-C	9.68	124.34	112.73
1	A	70	PHE	CA-CB-CG	7.76	121.56	113.80
2	E	35	LEU	CA-C-N	7.58	130.65	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	35	LEU	C-N-CA	7.58	130.65	120.65
2	B	35	LEU	CA-C-N	7.51	130.57	120.65
2	B	35	LEU	C-N-CA	7.51	130.57	120.65
1	D	70	PHE	CA-CB-CG	7.03	120.83	113.80
2	E	34	ALA	CA-C-O	-6.96	113.45	120.90
2	E	35	LEU	CA-C-O	-6.67	113.48	120.55
2	B	59	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	359	TYR	CA-C-N	6.31	125.94	121.65
1	A	359	TYR	C-N-CA	6.31	125.94	121.65
2	B	208	ASP	CA-CB-CG	6.03	118.63	112.60
1	D	359	TYR	CA-C-N	6.01	125.74	121.65
1	D	359	TYR	C-N-CA	6.01	125.74	121.65
2	B	52	ASP	CA-CB-CG	5.96	118.56	112.60
2	B	201	SER	CA-C-N	5.83	128.41	120.54
2	B	201	SER	C-N-CA	5.83	128.41	120.54
2	B	35	LEU	CA-C-O	-5.75	114.45	120.55
2	B	34	ALA	CA-C-O	-5.28	115.25	120.90
1	A	104	GLY	CA-C-N	5.21	131.49	121.54
1	A	104	GLY	C-N-CA	5.21	131.49	121.54
1	A	61	ASN	CA-CB-CG	5.15	117.75	112.60
2	E	132	SER	N-CA-C	-5.12	106.54	112.89
2	E	59	ASP	CA-CB-CG	5.06	117.66	112.60
2	E	34	ALA	O-C-N	5.02	127.31	122.09

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	3563	3517	3518	4	1
1	D	3563	3517	3520	4	0
2	B	1871	1923	1935	21	1
2	E	1809	1855	1867	15	0
3	C	23	22	21	0	0
3	F	23	22	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	30	33	32	0	0
4	E	30	33	33	0	0
5	B	1	0	0	0	0
6	A	3	0	0	0	0
6	B	8	0	0	1	0
6	D	13	0	0	0	0
6	E	7	0	0	0	0
All	All	10944	10922	10947	36	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 2.

All (36) 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)
2:B:35:LEU:CG	2:B:35:LEU:CB	1.93	1.47
2:E:35:LEU:CB	2:E:35:LEU:CG	1.92	1.45
2:B:35:LEU:HD22	2:E:38:ALA:HB3	1.69	0.74
2:B:193:LEU:CD1	2:B:233:PHE:CD1	2.75	0.68
2:E:35:LEU:CB	2:E:35:LEU:CD2	2.70	0.65
2:B:35:LEU:CB	2:B:35:LEU:CD2	2.73	0.63
2:B:193:LEU:HD13	2:B:233:PHE:CD1	2.37	0.59
2:B:193:LEU:CD1	2:B:233:PHE:CG	2.86	0.59
6:B:601:HOH:O	2:E:42:LEU:HD13	2.03	0.59
1:D:125:VAL:HG13	1:D:174:PRO:HA	1.84	0.58
1:A:125:VAL:HG13	1:A:174:PRO:HA	1.85	0.58
2:B:193:LEU:HD11	2:B:233:PHE:CE1	2.41	0.56
2:B:31:ALA:O	2:B:35:LEU:N	2.34	0.55
2:B:193:LEU:HD11	2:B:233:PHE:CD1	2.42	0.55
2:B:23:THR:HA	2:E:22:GLN:NE2	2.21	0.55
2:E:31:ALA:O	2:E:35:LEU:N	2.30	0.55
2:B:96:THR:HG21	2:E:71:ILE:HG12	1.89	0.55
1:A:372:SER:O	1:A:374:PRO:HD3	2.08	0.54
1:D:372:SER:O	1:D:374:PRO:HD3	2.09	0.53
2:E:115:PHE:CZ	2:E:119:ILE:HD11	2.44	0.53
2:B:57:MET:HA	2:B:57:MET:HE2	1.92	0.52
1:D:125:VAL:CG1	1:D:174:PRO:HA	2.43	0.49
1:A:125:VAL:CG1	1:A:174:PRO:HA	2.43	0.48
2:B:28:PHE:HE1	2:E:33:PHE:HB3	1.80	0.46
2:B:24:ARG:HH22	2:E:77:HIS:CE1	2.35	0.44
1:D:126:ILE:HG12	1:D:176:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HG12	1:A:176:ILE:HG13	1.99	0.43
2:B:22:GLN:O	2:E:22:GLN:OE1	2.37	0.42
2:E:155:ALA:O	2:E:159:VAL:HG23	2.19	0.42
2:B:103:LEU:CD1	2:E:37:ILE:HD12	2.49	0.42
2:B:103:LEU:HD11	2:E:37:ILE:HD12	2.03	0.41
2:B:154:PHE:CE1	2:B:199:LEU:HD13	2.56	0.41
2:B:230:MET:HA	2:B:230:MET:HE3	2.01	0.41
2:B:193:LEU:HD11	2:B:233:PHE:CG	2.56	0.41
2:B:193:LEU:HD11	2:B:233:PHE:CZ	2.56	0.41
2:E:46:ILE:N	2:E:46:ILE:HD12	2.36	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:HG	2:B:211:GLY:O[1_545]	1.58	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	456/486 (94%)	437 (96%)	18 (4%)	1 (0%)	43	73
1	D	456/486 (94%)	437 (96%)	18 (4%)	1 (0%)	43	73
2	B	228/255 (89%)	218 (96%)	9 (4%)	1 (0%)	30	62
2	E	220/255 (86%)	210 (96%)	8 (4%)	2 (1%)	14	47
All	All	1360/1482 (92%)	1302 (96%)	53 (4%)	5 (0%)	30	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	136	GLU
1	A	105	TRP
1	D	105	TRP
2	E	136	GLU
2	E	135	GLY

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	370/389 (95%)	368 (100%)	2 (0%)	81	85
1	D	370/389 (95%)	366 (99%)	4 (1%)	65	79
2	B	206/230 (90%)	198 (96%)	8 (4%)	28	62
2	E	199/230 (86%)	189 (95%)	10 (5%)	22	55
All	All	1145/1238 (92%)	1121 (98%)	24 (2%)	47	71

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	424	TYR
2	B	35	LEU
2	B	40	LEU
2	B	46	ILE
2	B	69	LEU
2	B	71	ILE
2	B	72	VAL
2	B	226	TYR
2	B	230	MET
1	D	31	ILE
1	D	51	VAL
1	D	71	THR
1	D	424	TYR
2	E	35	LEU
2	E	40	LEU
2	E	46	ILE

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Mol	Chain	Res	Type
2	E	59	ASP
2	E	69	LEU
2	E	71	ILE
2	E	72	VAL
2	E	104	VAL
2	E	109	LEU
2	E	156	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
2	B	139	HIS
2	B	140	GLN
2	B	148	ASN
2	B	191	ASN
1	D	61	ASN
1	D	135	ASN
2	E	139	HIS
2	E	191	ASN

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 ⓘ

4 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	C	1	3	12,12,12	1.26	2 (16%)	17,17,17	1.81	4 (23%)
3	GLC	C	2	3	11,11,12	1.72	2 (18%)	15,15,17	1.94	4 (26%)
3	GLC	F	1	3	12,12,12	1.21	0	17,17,17	1.86	5 (29%)
3	GLC	F	2	3	11,11,12	1.71	2 (18%)	15,15,17	1.98	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	C	1	3	-	0/2/22/22	0/1/1/1
3	GLC	C	2	3	-	0/2/19/22	0/1/1/1
3	GLC	F	1	3	-	0/2/22/22	0/1/1/1
3	GLC	F	2	3	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	GLC	O5-C1	-3.97	1.37	1.43
3	F	2	GLC	O5-C1	-3.94	1.37	1.43
3	C	2	GLC	O2-C2	-2.51	1.38	1.43
3	F	2	GLC	O2-C2	-2.43	1.38	1.43
3	C	1	GLC	O3-C3	-2.14	1.37	1.43
3	C	1	GLC	O5-C5	-2.06	1.39	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	GLC	C1-O5-C5	5.03	118.92	112.19
3	C	2	GLC	C1-O5-C5	4.90	118.75	112.19
3	C	1	GLC	O5-C1-C2	3.98	117.30	110.30
3	C	1	GLC	C1-O5-C5	3.96	121.31	113.65
3	F	1	GLC	O5-C1-C2	3.96	117.25	110.30
3	F	1	GLC	C1-O5-C5	3.91	121.22	113.65
3	F	2	GLC	O5-C5-C6	-3.78	100.30	107.66
3	C	2	GLC	O5-C5-C6	-3.65	100.56	107.66
3	F	2	GLC	O3-C3-C4	-2.65	104.13	110.38
3	C	2	GLC	O3-C3-C4	-2.63	104.17	110.38
3	C	2	GLC	O3-C3-C2	2.42	114.99	110.05
3	F	1	GLC	O5-C5-C6	-2.25	100.87	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	GLC	O5-C5-C6	-2.22	100.95	106.44
3	F	2	GLC	O3-C3-C2	2.19	114.52	110.05
3	F	1	GLC	O2-C2-C1	2.14	114.20	109.25
3	C	1	GLC	O2-C2-C1	2.05	113.99	109.25
3	F	1	GLC	C4-C3-C2	-2.01	107.30	110.83

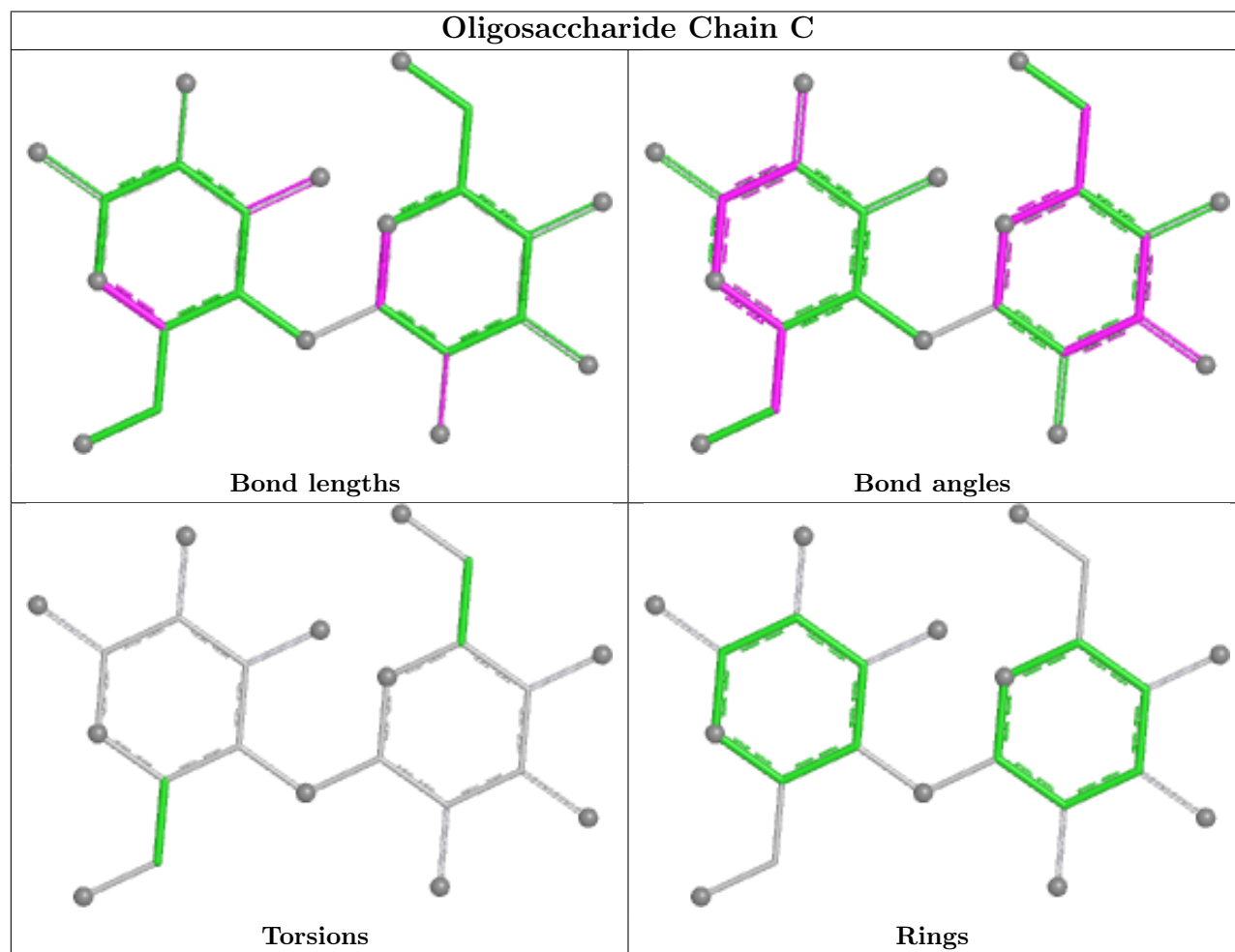
There are no chirality outliers.

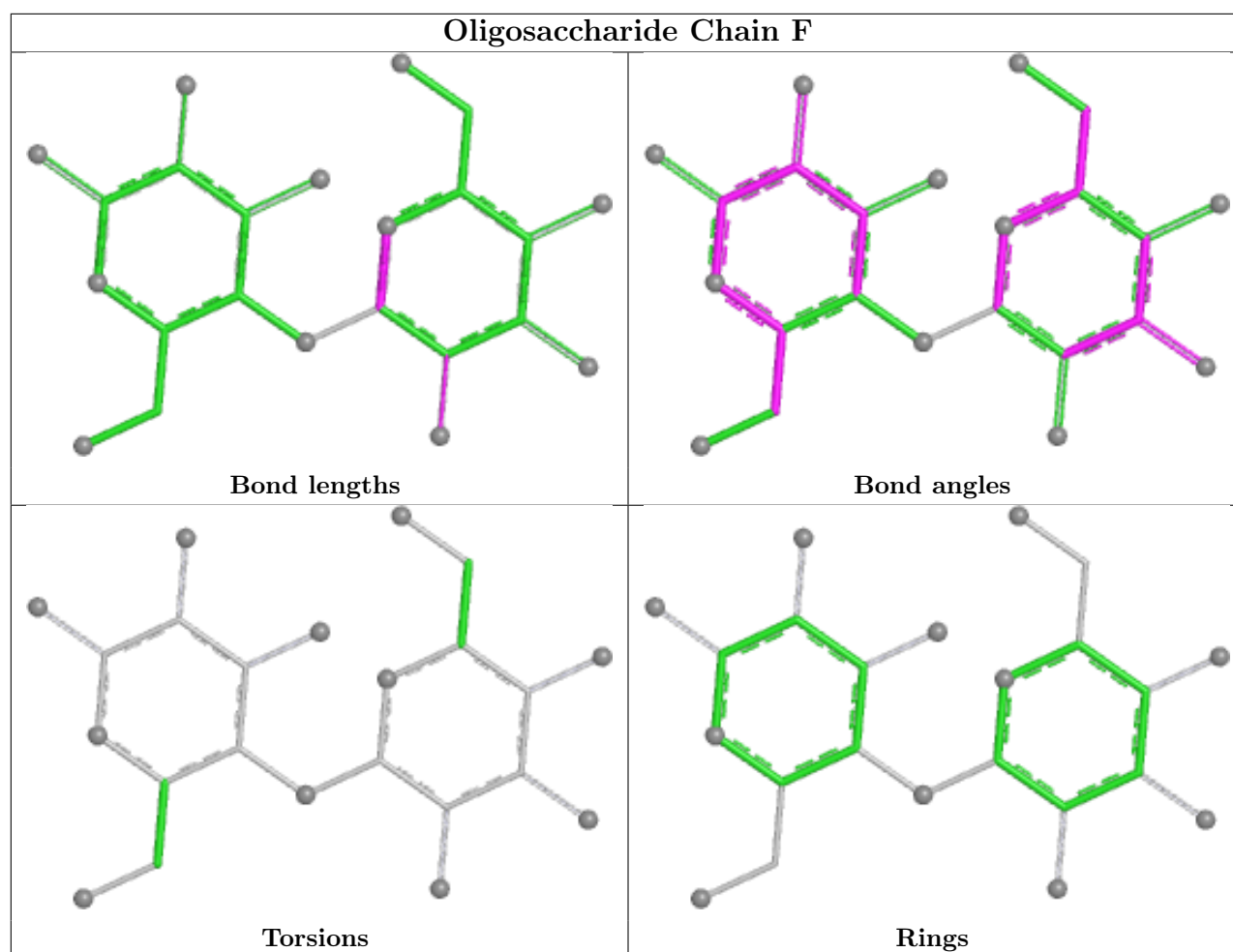
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	LMT	B	501	-	31,31,36	1.10	3 (9%)	42,42,47	1.42	9 (21%)
4	LMT	E	501	-	31,31,36	1.17	3 (9%)	42,42,47	1.57	7 (16%)

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	LMT	B	501	-	-	4/16/56/61	0/2/2/2
4	LMT	E	501	-	-	5/16/56/61	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	501	LMT	C3'-C4'	2.39	1.58	1.52
4	B	501	LMT	C4B-C3B	2.26	1.58	1.52
4	B	501	LMT	O1'-C1'	2.16	1.43	1.40
4	E	501	LMT	C4B-C5B	2.09	1.57	1.53
4	E	501	LMT	C4'-C5'	2.08	1.58	1.52
4	B	501	LMT	O2'-C2'	-2.01	1.38	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	501	LMT	C1B-O5B-C5B	4.77	123.04	113.72
4	E	501	LMT	C1'-C2'-C3'	-3.26	103.14	110.01
4	B	501	LMT	O2B-C2B-C3B	-3.07	103.15	110.38
4	E	501	LMT	C3B-C4B-C5B	-2.99	104.80	110.23
4	B	501	LMT	O4'-C4B-C5B	-2.90	102.17	109.32
4	E	501	LMT	C4B-C3B-C2B	-2.75	106.01	110.83
4	E	501	LMT	O1B-C4'-C5'	-2.61	102.63	109.48
4	B	501	LMT	C4B-C3B-C2B	2.58	115.37	110.83
4	B	501	LMT	O5'-C1'-C2'	-2.35	105.55	110.37
4	B	501	LMT	O3B-C3B-C4B	-2.26	105.06	110.38
4	E	501	LMT	O5B-C1B-C2B	2.25	114.99	110.37
4	E	501	LMT	O5'-C1'-C2'	-2.20	105.85	110.37
4	B	501	LMT	C1B-O5B-C5B	2.15	117.91	113.72
4	B	501	LMT	O2B-C2B-C1B	2.10	115.09	110.08
4	B	501	LMT	O5'-C5'-C4'	2.08	114.03	109.72
4	B	501	LMT	C1B-C2B-C3B	2.05	114.33	110.01

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	LMT	O5'-C5'-C6'-O6'
4	E	501	LMT	O5'-C5'-C6'-O6'

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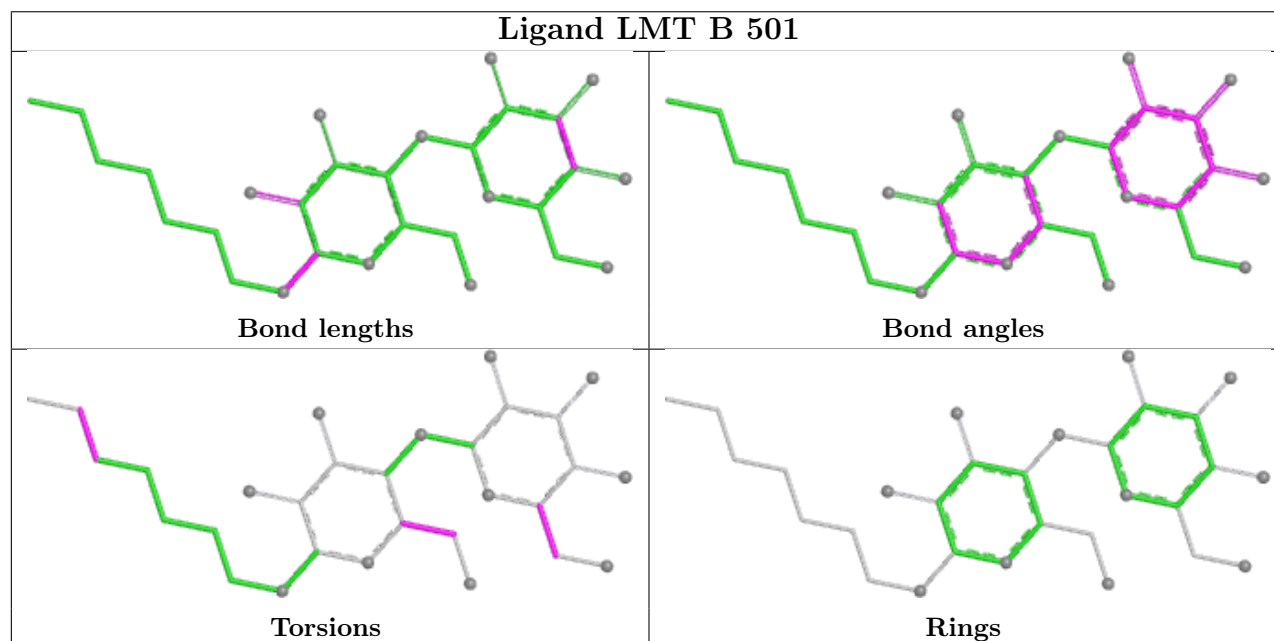
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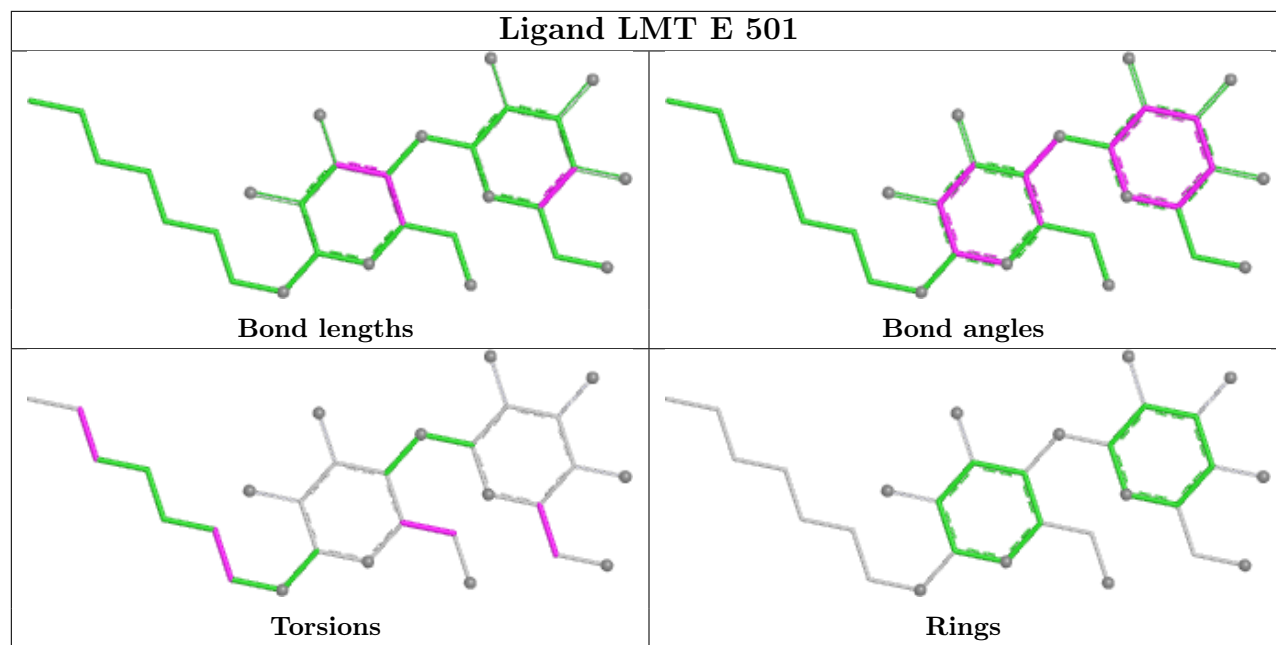
Mol	Chain	Res	Type	Atoms
4	E	501	LMT	C4'-C5'-C6'-O6'
4	E	501	LMT	O1'-C1-C2-C3
4	B	501	LMT	C4'-C5'-C6'-O6'
4	E	501	LMT	O5B-C5B-C6B-O6B
4	B	501	LMT	O5B-C5B-C6B-O6B
4	B	501	LMT	C4-C5-C6-C7
4	E	501	LMT	C4-C5-C6-C7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	460/486 (94%)	0.08	27 (5%)	28 18	189, 244, 271, 291	0
1	D	460/486 (94%)	-0.05	25 (5%)	31 20	181, 245, 268, 281	0
2	B	230/255 (90%)	0.40	22 (9%)	13 9	37, 192, 260, 271	0
2	E	222/255 (87%)	0.31	10 (4%)	38 24	44, 187, 237, 258	0
All	All	1372/1482 (92%)	0.13	84 (6%)	27 17	37, 234, 266, 291	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	233	PHE	6.7
2	B	119	ILE	5.8
2	B	9	VAL	5.2
1	A	240	PRO	4.9
2	E	9	VAL	4.8
2	E	173	LEU	4.8
1	D	274	THR	4.8
1	A	412	LYS	4.7
1	A	243	PRO	4.6
1	D	383	ILE	4.6
2	E	170	MET	4.4
1	D	416	LEU	4.3
1	A	241	ASN	4.3
2	B	123	ILE	4.2
1	D	209	PHE	4.2
1	A	11	GLY	3.9
1	A	23	LEU	3.9
2	B	232	VAL	3.8
1	A	96	TYR	3.8
2	E	26	GLU	3.6
1	A	72	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	83	LEU	3.3
1	D	128	ILE	3.2
2	B	11	LEU	3.2
1	A	252	LEU	3.1
1	D	243	PRO	3.1
1	D	464	VAL	3.1
1	A	278	ILE	3.0
2	B	228	PRO	3.0
1	D	241	ASN	3.0
1	A	36	ARG	3.0
1	D	229	ALA	3.0
2	B	38	ALA	2.9
1	A	282	GLY	2.8
1	A	21	LEU	2.8
1	D	412	LYS	2.8
1	A	12	GLY	2.8
1	D	240	PRO	2.7
1	A	340	ALA	2.6
2	B	99	LEU	2.6
2	B	104	VAL	2.6
1	A	209	PHE	2.6
1	A	411	ASN	2.6
1	D	411	ASN	2.6
1	D	178	PHE	2.5
2	B	225	LEU	2.5
1	D	228	GLU	2.5
1	D	210	THR	2.5
1	D	278	ILE	2.5
1	A	238	LEU	2.5
1	D	417	GLY	2.5
2	B	130	ASP	2.5
2	B	120	TYR	2.5
2	B	209	PRO	2.5
1	A	228	GLU	2.4
2	B	131	LEU	2.4
1	A	29	GLY	2.4
2	B	24	ARG	2.4
1	A	263	ALA	2.4
1	D	247	GLU	2.4
1	D	20	SER	2.4
2	E	72	VAL	2.4
2	B	33	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	111	ASP	2.3
1	A	6	GLN	2.3
2	B	78	TYR	2.3
1	D	21	LEU	2.3
1	A	242	PRO	2.2
1	D	272	TYR	2.2
1	D	15	VAL	2.2
2	E	222	LEU	2.2
2	B	34	ALA	2.2
2	B	179	TYR	2.1
2	B	230	MET	2.1
1	D	410	VAL	2.1
2	B	226	TYR	2.1
2	E	137	TYR	2.1
1	A	229	ALA	2.1
2	E	86	LEU	2.1
1	A	39	TRP	2.0
1	A	341	MET	2.0
1	D	194	ALA	2.0
2	E	135	GLY	2.0
2	E	229	ILE	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 ⓘ

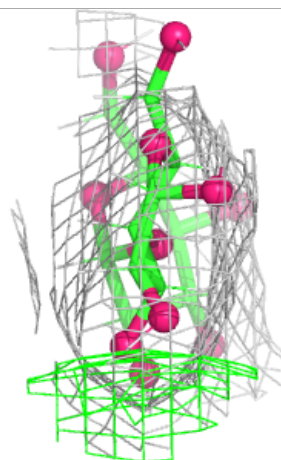
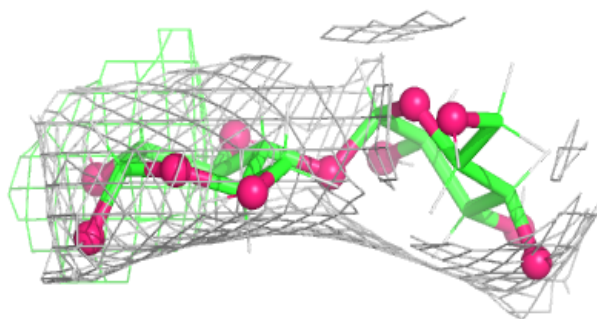
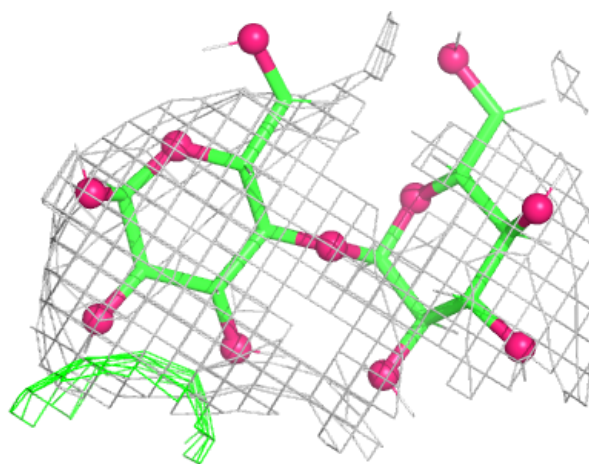
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

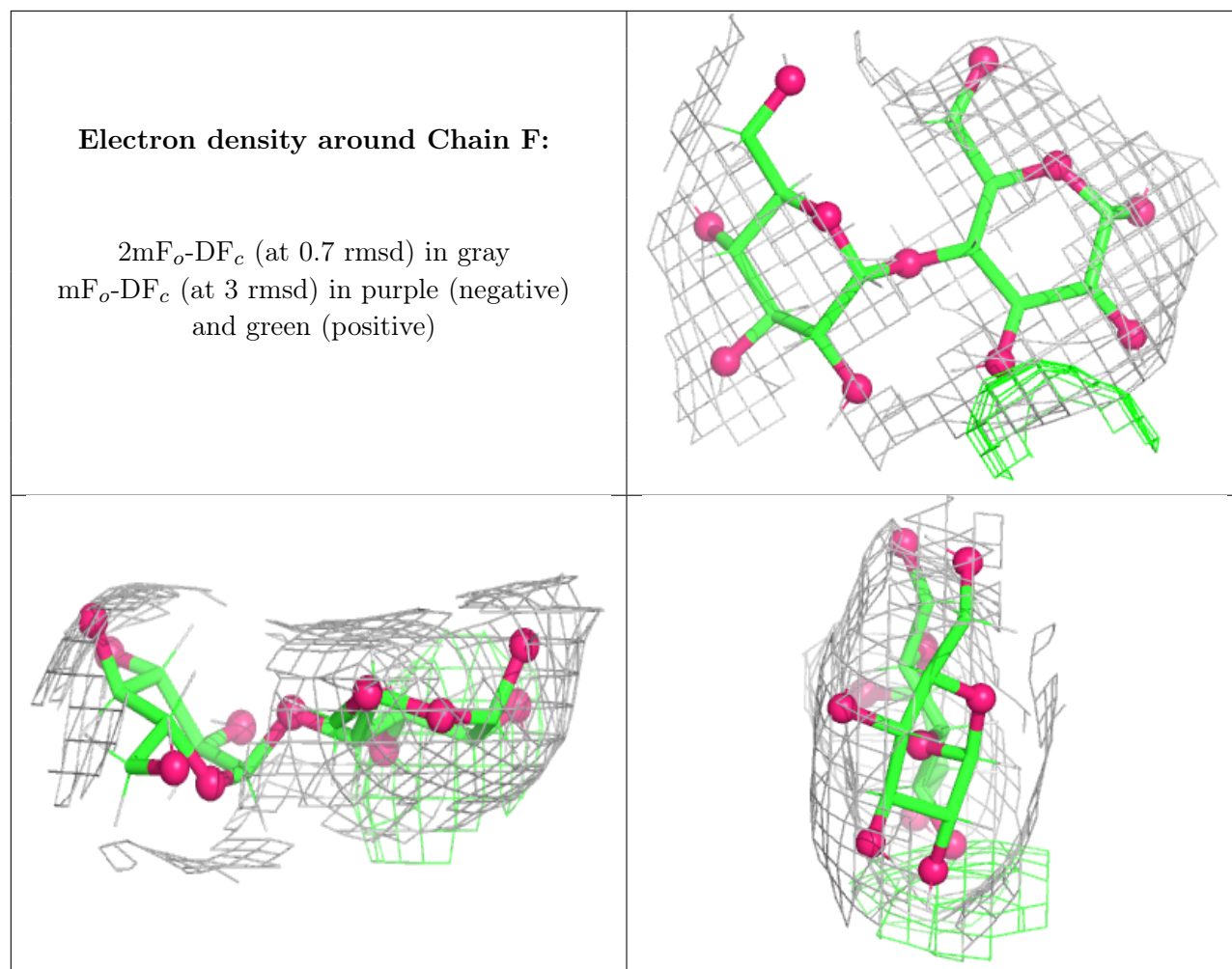
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	C	1	12/12	-	-	184,187,188,188	0
3	GLC	C	2	11/12	-	-	191,194,198,199	0
3	GLC	F	1	12/12	0.72	0.11	176,178,180,184	0
3	GLC	F	2	11/12	0.87	0.06	187,190,191,192	0

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 C:

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





6.4 Ligands [i](#)

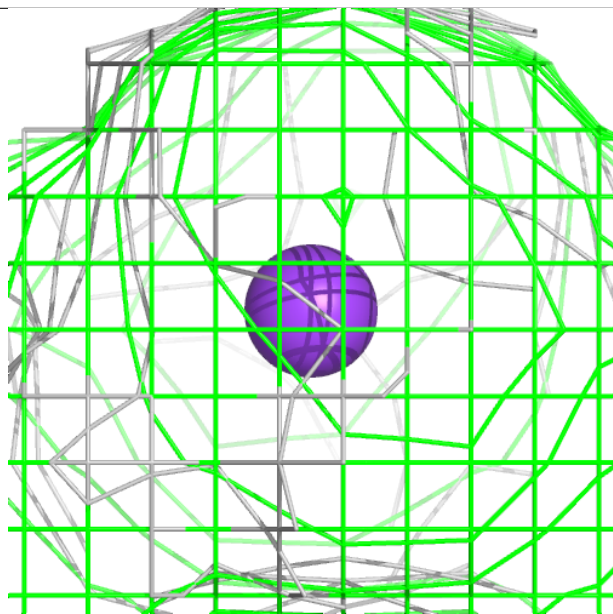
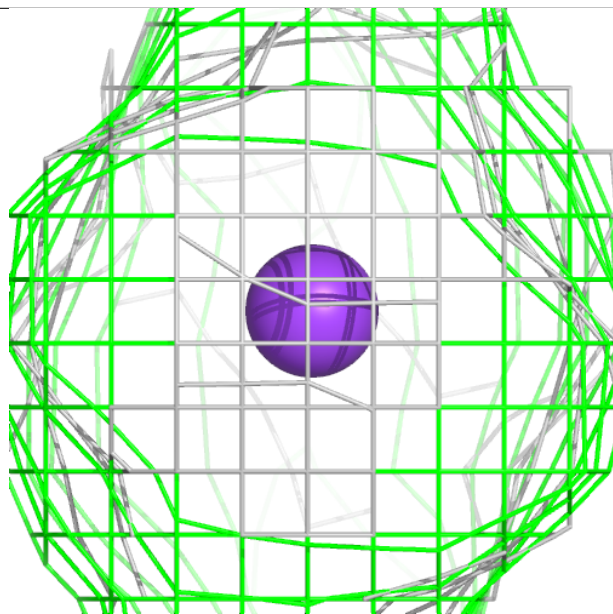
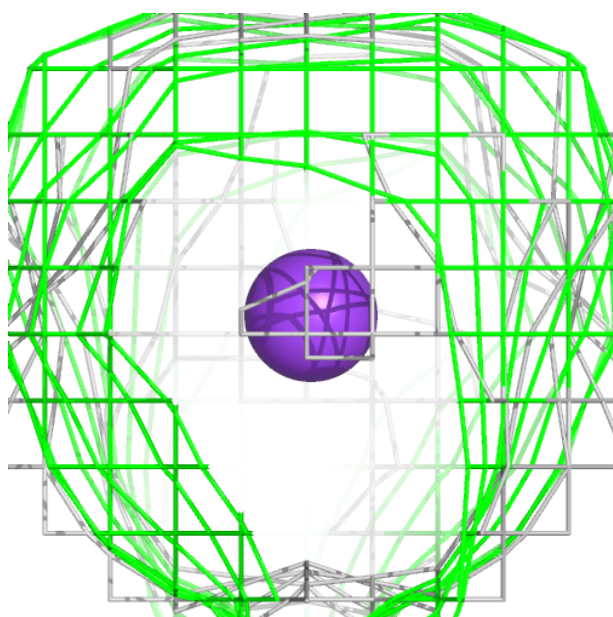
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	K	B	502	1/1	0.16	0.53	251,251,251,251	1
4	LMT	B	501	30/35	0.80	0.11	209,218,230,230	0
4	LMT	E	501	30/35	0.88	0.11	194,198,210,211	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

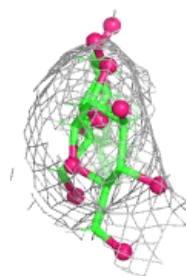
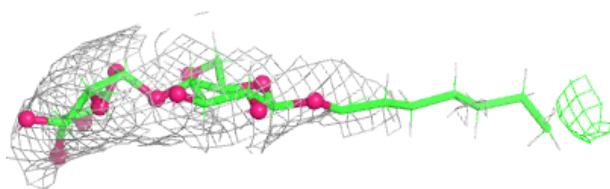
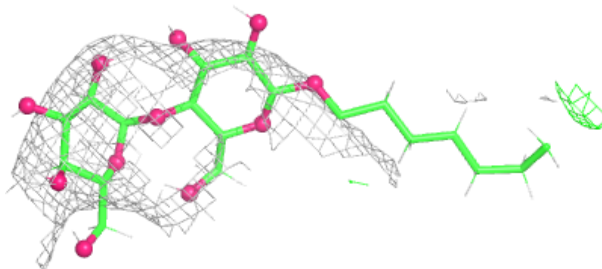
Electron density around K B 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

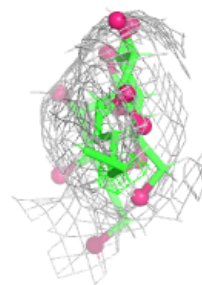
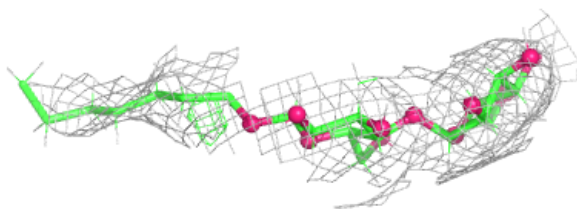
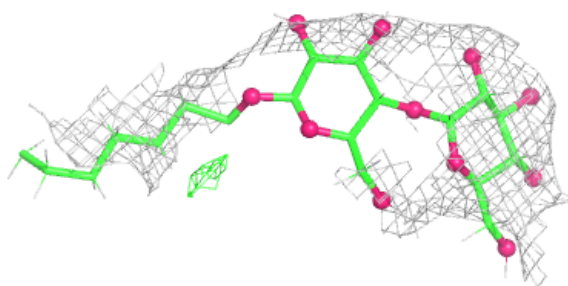


Electron density around LMT B 501:

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

**Electron density around LMT E 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.