



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:42 PM UTC

PDB ID : 3MP1 / pdb_00003mp1
Title : Complex structure of Sgf29 and trimethylated H3K4
Authors : Li, J.; Ruan, J.; Wu, M.; Xue, X.; Zang, J.
Deposited on : 2010-04-24
Resolution : 2.60 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
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

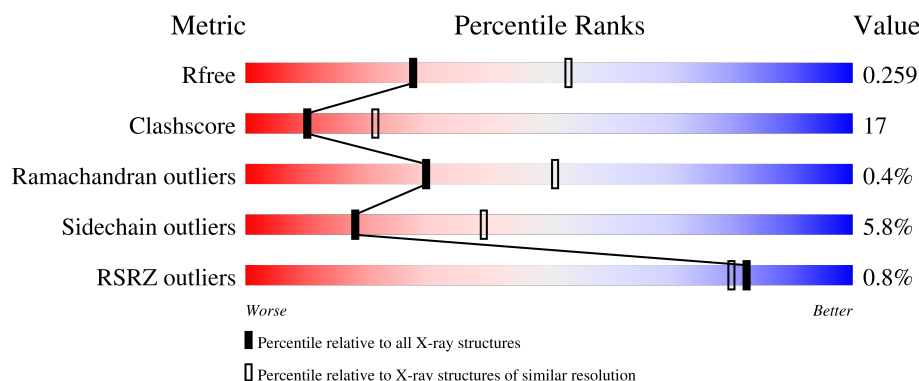
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	522	% 64% 30% • •
2	P	5	60% 40%
3	B	2	50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4295 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-binding periplasmic protein, LINKER, SAGA-associated factor 29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	4	0	0
			3961	2544	654	753	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	738	MET	-	initiating methionine	UNP P0AEX9

- Molecule 2 is a protein called H3K4me3 peptide.

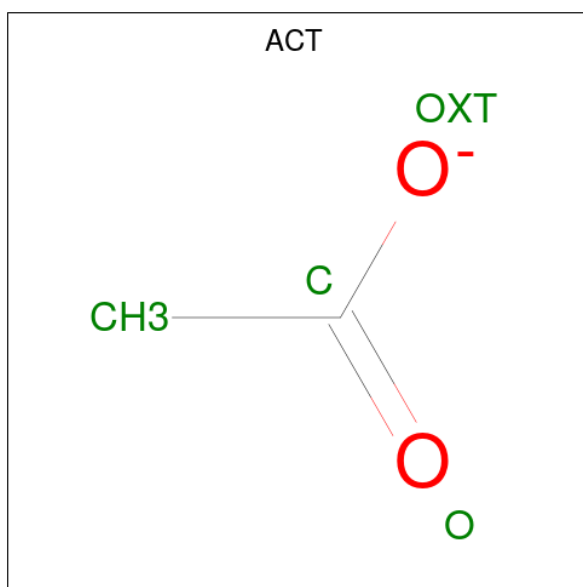
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	5	Total	C	N	O	0	0	0
			44	27	10	7			

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



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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

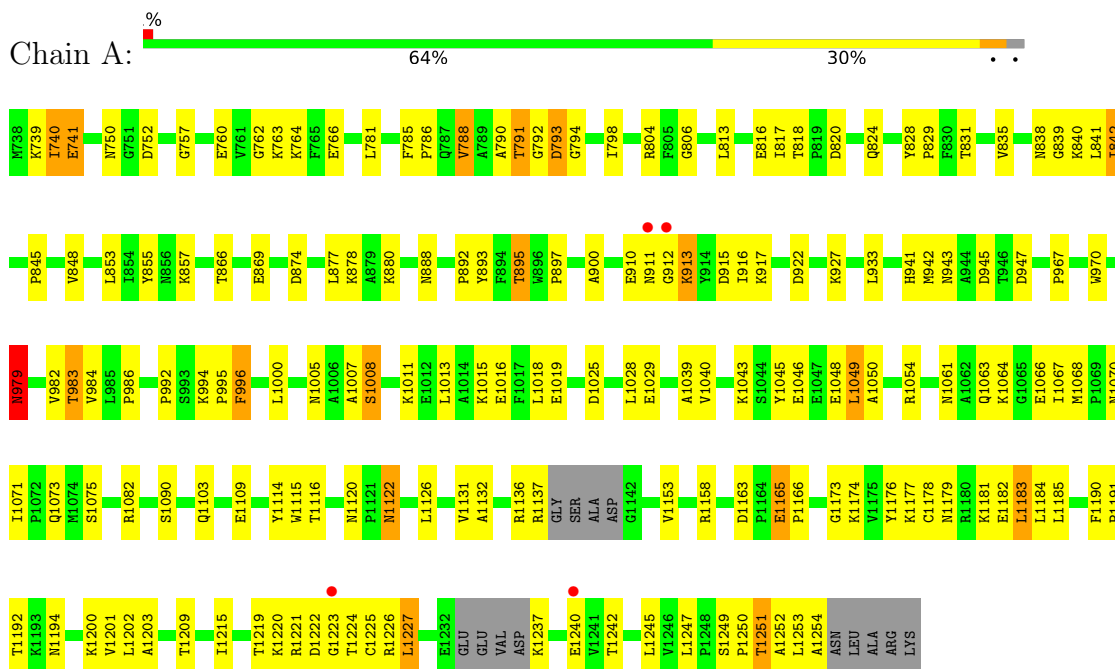
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	262	Total	O	0	0
			262	262		
5	P	1	Total	O	0	0
			1	1		

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: Maltose-binding periplasmic protein, LINKER, SAGA-associated factor 29



- Molecule 2: H3K4me3 peptide



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.24Å 84.84Å 119.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 2.60 48.76 – 2.61	Depositor EDS
% Data completeness (in resolution range)	94.5 (48.76-2.60) 94.6 (48.76-2.61)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.66 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.223 , 0.260 0.219 , 0.259	Depositor DCC
R_{free} test set	757 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 24.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4295	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: ACT, GLC, M3L

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	0.49	0/4058	0.98	17/5513 (0.3%)
2	P	0.52	0/31	0.80	0/40
All	All	0.49	0/4089	0.98	17/5553 (0.3%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	913	LYS	N-CA-C	10.04	121.10	108.45
1	A	1018	LEU	N-CA-C	6.92	118.61	111.14
1	A	979	ASN	N-CA-C	-6.20	97.09	107.99
1	A	1165	GLU	CA-C-N	6.04	127.39	119.84
1	A	1165	GLU	C-N-CA	6.04	127.39	119.84
1	A	910	GLU	N-CA-C	5.94	123.46	110.80
1	A	1209	THR	N-CA-C	-5.93	104.58	112.94
1	A	1013	LEU	N-CA-C	-5.84	104.87	112.23
1	A	1008	SER	N-CA-C	5.52	116.85	109.83
1	A	912	GLY	N-CA-C	-5.35	100.50	113.18
1	A	1227	LEU	N-CA-C	5.31	117.47	109.23
1	A	941	HIS	N-CA-C	-5.27	107.02	113.50
1	A	818	THR	N-CA-C	5.20	118.11	109.79
1	A	1000	LEU	N-CA-C	-5.19	102.71	110.23
1	A	1040	VAL	N-CA-C	5.10	116.15	109.21
1	A	855	TYR	N-CA-C	5.09	117.41	109.52
1	A	842	ILE	N-CA-C	5.08	117.00	112.17

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	3961	0	3927	136	0
2	P	44	0	54	2	0
3	B	23	0	21	1	0
4	A	4	0	3	0	0
5	A	262	0	0	31	0
5	P	1	0	0	0	0
All	All	4295	0	4005	138	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 17.

All (138) 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:1215:ILE:HD11	5:A:278:HOH:O	1.60	1.01
1:A:880:LYS:HE2	5:A:137:HOH:O	1.65	0.96
1:A:740:ILE:HD12	1:A:740:ILE:H	1.27	0.95
1:A:793:ASP:OD1	1:A:794:GLY:N	2.05	0.90
1:A:790:ALA:HB3	5:A:229:HOH:O	1.78	0.84
1:A:1220:LYS:NZ	1:A:1240:GLU:OE1	2.12	0.82
1:A:895:THR:HG21	1:A:933:LEU:HD22	1.63	0.79
1:A:790:ALA:CB	5:A:229:HOH:O	2.31	0.79
1:A:790:ALA:C	1:A:792:GLY:H	1.90	0.77
1:A:1090:SER:HB3	5:A:254:HOH:O	1.83	0.76
1:A:762:GLY:O	1:A:766:GLU:HG3	1.86	0.76
1:A:895:THR:CG2	1:A:933:LEU:HD22	2.18	0.73
1:A:1066:GLU:OE2	5:A:294:HOH:O	2.04	0.73
1:A:1153:VAL:HG23	1:A:1158:ARG:HB3	1.71	0.73
1:A:740:ILE:H	1:A:740:ILE:CD1	2.02	0.73
1:A:945:ASP:HB2	5:A:234:HOH:O	1.87	0.72
1:A:1116:THR:HG22	1:A:1122:ASN:OD1	1.89	0.72
1:A:829:PRO:HG3	5:A:269:HOH:O	1.90	0.71
1:A:740:ILE:HD12	1:A:740:ILE:N	2.04	0.71
1:A:857:LYS:HB2	1:A:979:ASN:ND2	2.07	0.69
1:A:915:ASP:OD1	1:A:917:LYS:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1190:PHE:CD1	1:A:1191:PRO:HD2	2.29	0.68
1:A:1249:SER:O	1:A:1253:LEU:HG	1.93	0.67
1:A:790:ALA:C	1:A:792:GLY:N	2.46	0.65
1:A:1005:ASN:HD21	1:A:1007:ALA:HB3	1.63	0.63
1:A:970:TRP:CH2	1:A:1054:ARG:HB3	2.33	0.63
1:A:1221:ARG:C	1:A:1223:GLY:H	2.06	0.63
1:A:790:ALA:O	1:A:792:GLY:N	2.32	0.63
1:A:943:ASN:HB3	5:A:234:HOH:O	1.99	0.63
1:A:1178:CYS:HB2	1:A:1182:GLU:HB2	1.81	0.62
1:A:1158:ARG:NH2	5:A:53:HOH:O	2.34	0.61
1:A:838:ASN:N	5:A:286:HOH:O	2.30	0.61
1:A:1200:LYS:HD2	1:A:1252:ALA:HB2	1.82	0.60
1:A:983:THR:OG1	1:A:984:VAL:N	2.32	0.60
1:A:1184:LEU:HD11	1:A:1250:PRO:HG3	1.84	0.59
2:P:4:M3L:HG3	2:P:5:GLN:N	2.19	0.58
1:A:785:PHE:HB3	1:A:786:PRO:HD3	1.86	0.57
1:A:1008:SER:O	1:A:1011:LYS:NZ	2.38	0.57
1:A:1165:GLU:OE1	1:A:1166:PRO:HD2	2.06	0.56
1:A:1016:GLU:HG2	5:A:51:HOH:O	2.05	0.56
1:A:828:TYR:HB2	1:A:831:THR:HG23	1.89	0.55
1:A:804:ARG:HH12	1:A:1075:SER:HB3	1.71	0.55
1:A:741:GLU:OE1	1:A:741:GLU:N	2.24	0.54
1:A:877:LEU:O	1:A:880:LYS:HG2	2.08	0.54
1:A:1184:LEU:HD11	1:A:1250:PRO:CG	2.36	0.54
1:A:806:GLY:HA3	1:A:1070:ASN:O	2.07	0.54
1:A:1221:ARG:C	1:A:1223:GLY:N	2.62	0.53
1:A:788:VAL:O	1:A:791:THR:HG22	2.08	0.53
1:A:1114:TYR:CE2	1:A:1181:LYS:HE3	2.43	0.53
1:A:1136:ARG:NH1	5:A:73:HOH:O	2.41	0.53
1:A:839:GLY:N	5:A:271:HOH:O	2.22	0.53
1:A:1082:ARG:NH2	5:A:75:HOH:O	2.43	0.52
1:A:994:LYS:HE2	5:A:161:HOH:O	2.08	0.52
1:A:1177:LYS:HD3	5:A:41:HOH:O	2.08	0.52
1:A:1225:CYS:HB3	1:A:1227:LEU:HD21	1.91	0.52
1:A:793:ASP:OD1	1:A:793:ASP:C	2.52	0.51
1:A:1163:ASP:O	1:A:1173:GLY:HA3	2.10	0.51
1:A:835:VAL:O	1:A:842:ILE:HG12	2.10	0.51
1:A:1221:ARG:O	1:A:1223:GLY:N	2.43	0.51
1:A:1174:LYS:HD3	1:A:1176:TYR:CZ	2.46	0.51
1:A:1190:PHE:HB3	5:A:306:HOH:O	2.09	0.51
1:A:838:ASN:HA	5:A:286:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1067:ILE:N	1:A:1067:ILE:HD12	2.26	0.50
1:A:835:VAL:HG21	1:A:845:PRO:HD3	1.93	0.50
1:A:1025:ASP:O	1:A:1029:GLU:HB2	2.12	0.50
1:A:1194:ASN:OD1	1:A:1219:THR:HG21	2.11	0.50
1:A:1103:GLN:NE2	5:A:242:HOH:O	2.33	0.50
1:A:1174:LYS:HD3	1:A:1176:TYR:OH	2.13	0.49
1:A:1190:PHE:CD1	1:A:1191:PRO:CD	2.96	0.49
1:A:984:VAL:HA	1:A:1061:ASN:HD21	1.77	0.49
1:A:888:ASN:ND2	1:A:947:ASP:HA	2.27	0.49
1:A:1015:LYS:HE3	1:A:1019:GLU:OE2	2.13	0.49
1:A:1184:LEU:CD1	1:A:1202:LEU:HD12	2.42	0.49
1:A:1226:ARG:O	1:A:1227:LEU:HD23	2.12	0.49
1:A:853:LEU:HD22	1:A:986:PRO:HD3	1.93	0.49
1:A:1201:VAL:HB	1:A:1247:LEU:O	2.13	0.49
2:P:4:M3L:HG3	2:P:5:GLN:H	1.78	0.49
1:A:892:PRO:HD3	1:A:1082:ARG:HG3	1.95	0.49
1:A:820:ASP:O	1:A:824:GLN:HG3	2.13	0.48
1:A:1190:PHE:CB	5:A:306:HOH:O	2.61	0.48
1:A:874:ASP:O	1:A:878:LYS:HG2	2.13	0.48
1:A:1254:ALA:HB2	5:A:190:HOH:O	2.13	0.48
1:A:813:LEU:HD23	1:A:813:LEU:N	2.28	0.48
1:A:943:ASN:CB	5:A:234:HOH:O	2.59	0.48
1:A:750:ASN:ND2	1:A:752:ASP:OD1	2.46	0.47
1:A:1132:ALA:O	1:A:1183:LEU:HA	2.14	0.47
1:A:816:GLU:OE2	1:A:840:LYS:HG2	2.14	0.47
1:A:893:TYR:HB2	3:B:2:GLC:O5	2.14	0.47
1:A:763:LYS:HE2	5:A:183:HOH:O	2.14	0.47
1:A:853:LEU:HD22	1:A:986:PRO:HG3	1.96	0.47
1:A:804:ARG:NH1	1:A:1075:SER:HB3	2.29	0.47
1:A:1194:ASN:CG	1:A:1219:THR:HG21	2.40	0.46
1:A:1122:ASN:H	1:A:1122:ASN:HD22	1.63	0.46
1:A:817:ILE:HD11	1:A:841:LEU:HB3	1.97	0.46
1:A:900:ALA:HB1	1:A:994:LYS:HZ2	1.81	0.46
1:A:741:GLU:H	1:A:741:GLU:CD	2.13	0.46
1:A:1028:LEU:HD23	1:A:1028:LEU:HA	1.71	0.46
1:A:996:PHE:CG	1:A:1068:MET:HG2	2.51	0.45
1:A:1254:ALA:CB	5:A:190:HOH:O	2.65	0.45
1:A:1029:GLU:HA	1:A:1045:TYR:OH	2.16	0.45
1:A:922:ASP:O	1:A:927:LYS:HE2	2.15	0.45
1:A:1043:LYS:HE3	5:A:230:HOH:O	2.17	0.45
1:A:1073:GLN:OE1	1:A:1073:GLN:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:GLU:HB3	5:A:307:HOH:O	2.17	0.44
1:A:1049:LEU:HD23	1:A:1049:LEU:N	2.32	0.44
1:A:1064:LYS:HG3	5:A:70:HOH:O	2.16	0.44
1:A:933:LEU:HD11	1:A:942:MET:HE1	1.99	0.44
1:A:785:PHE:CG	1:A:798:ILE:HD12	2.52	0.44
1:A:804:ARG:HH12	1:A:1075:SER:CB	2.31	0.44
1:A:757:GLY:O	1:A:760:GLU:HB2	2.18	0.43
1:A:1179:ASN:OD1	1:A:1182:GLU:HG3	2.17	0.43
1:A:1131:VAL:HG12	1:A:1185:LEU:HA	1.99	0.43
1:A:1190:PHE:N	5:A:306:HOH:O	2.51	0.43
1:A:838:ASN:CA	5:A:286:HOH:O	2.61	0.43
1:A:1136:ARG:HH21	1:A:1136:ARG:HG2	1.84	0.43
1:A:1067:ILE:N	1:A:1067:ILE:CD1	2.81	0.43
1:A:848:VAL:HB	1:A:1039:ALA:HB3	2.02	0.42
1:A:781:LEU:HD12	1:A:781:LEU:C	2.44	0.42
1:A:1249:SER:OG	1:A:1251:THR:HG23	2.19	0.42
1:A:785:PHE:N	1:A:786:PRO:CD	2.83	0.42
1:A:992:PRO:O	5:A:232:HOH:O	2.21	0.42
1:A:739:LYS:HB3	1:A:741:GLU:OE1	2.20	0.42
1:A:853:LEU:HD22	1:A:986:PRO:CG	2.50	0.42
1:A:866:THR:OG1	1:A:869:GLU:HG3	2.19	0.41
1:A:1114:TYR:CD2	1:A:1181:LYS:HE3	2.55	0.41
1:A:1203:ALA:HA	1:A:1245:LEU:O	2.21	0.41
1:A:897:PRO:HG3	1:A:995:PRO:HA	2.02	0.41
1:A:1046:GLU:O	1:A:1050:ALA:HB2	2.20	0.41
1:A:916:ILE:HG22	1:A:1071:ILE:HD12	2.01	0.41
1:A:878:LYS:HD3	1:A:878:LYS:HA	1.88	0.41
1:A:1122:ASN:C	1:A:1122:ASN:ND2	2.78	0.41
1:A:816:GLU:OE1	1:A:840:LYS:HE2	2.20	0.41
1:A:1115:TRP:CE2	1:A:1250:PRO:HB3	2.56	0.41
1:A:967:PRO:HA	1:A:970:TRP:CE2	2.56	0.41
1:A:982:VAL:CG2	1:A:1054:ARG:HG2	2.51	0.41
1:A:1190:PHE:HA	1:A:1191:PRO:HD3	1.83	0.41
1:A:764:LYS:HA	1:A:764:LYS:HD2	1.95	0.40
1:A:1153:VAL:CG2	1:A:1158:ARG:HB3	2.47	0.40

There are no symmetry-related clashes.

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	503/522 (96%)	479 (95%)	22 (4%)	2 (0%)	30	51
2	P	2/5 (40%)	2 (100%)	0	0	100	100
All	All	505/527 (96%)	481 (95%)	22 (4%)	2 (0%)	30	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	791	THR
1	A	1222	ASP

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	413/423 (98%)	389 (94%)	24 (6%)	18	39
2	P	3/3 (100%)	3 (100%)	0	100	100
All	All	416/426 (98%)	392 (94%)	24 (6%)	18	39

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

Mol	Chain	Res	Type
1	A	740	ILE
1	A	741	GLU
1	A	788	VAL
1	A	793	ASP

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Mol	Chain	Res	Type
1	A	895	THR
1	A	911	ASN
1	A	913	LYS
1	A	979	ASN
1	A	983	THR
1	A	996	PHE
1	A	1048	GLU
1	A	1049	LEU
1	A	1063	GLN
1	A	1109	GLU
1	A	1120	ASN
1	A	1122	ASN
1	A	1126	LEU
1	A	1137	ARG
1	A	1183	LEU
1	A	1192	THR
1	A	1224	THR
1	A	1237	LYS
1	A	1242	THR
1	A	1251	THR

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

Mol	Chain	Res	Type
1	A	810	GLN
1	A	838	ASN
1	A	862	ASN
1	A	888	ASN
1	A	911	ASN
1	A	956	ASN
1	A	1005	ASN
1	A	1087	ASN
1	A	1120	ASN
1	A	1122	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	M3L	P	4	2	10,11,12	0.63	0	9,14,16	1.19	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
2	M3L	P	4	2	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	4	M3L	2	0

5.5 Carbohydrates ⓘ

2 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	B	1	3	12,12,12	0.86	0	17,17,17	0.87	1 (5%)
3	GLC	B	2	3	11,11,12	1.33	2 (18%)	15,15,17	0.88	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	B	1	3	-	0/2/22/22	0/1/1/1
3	GLC	B	2	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	GLC	O5-C1	2.33	1.47	1.43
3	B	2	GLC	O5-C5	2.08	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	GLC	C4-C3-C2	-2.13	107.09	110.83

There are no chirality outliers.

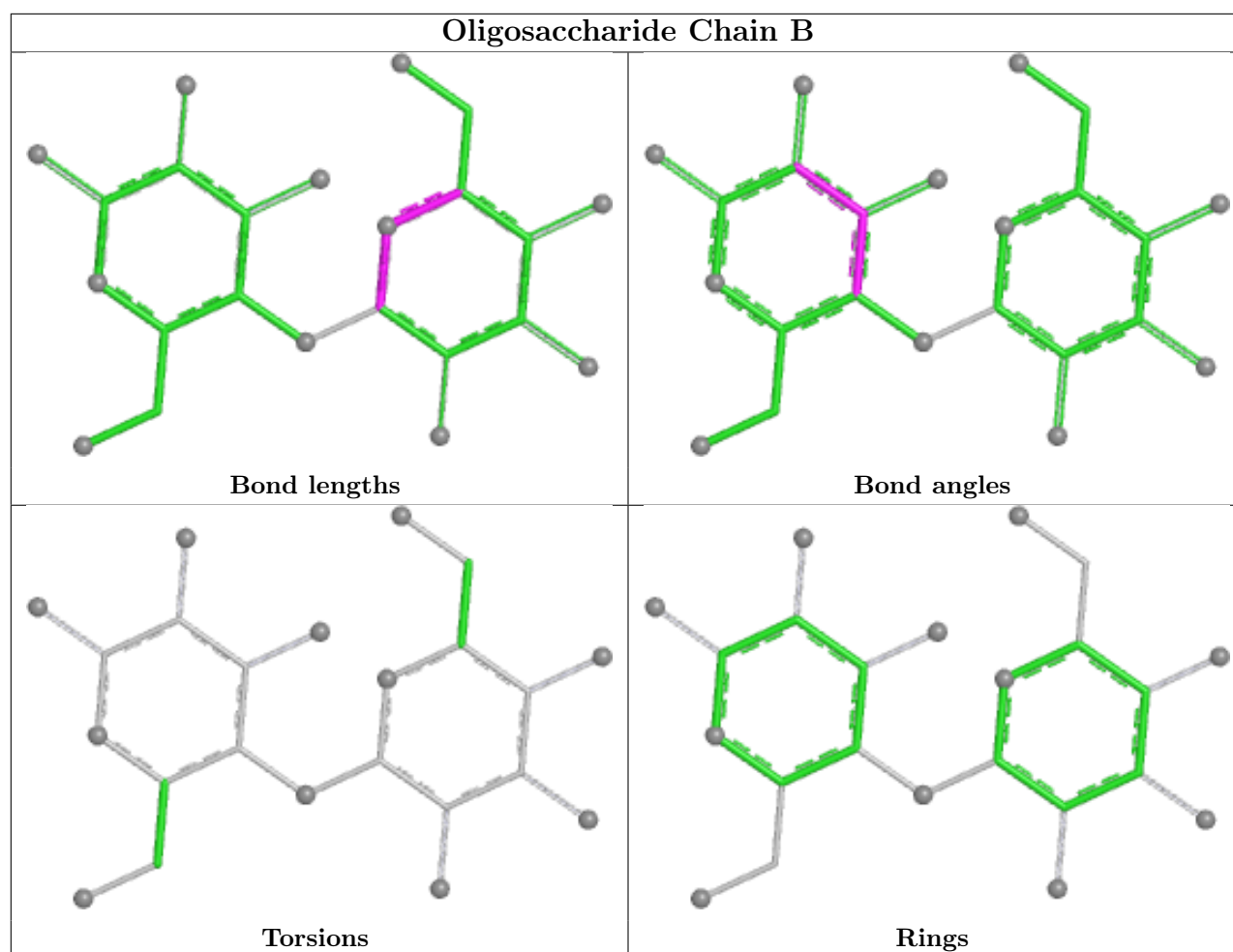
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	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](#)

1 ligand is 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	ACT	A	1	-	3,3,3	1.23	0	3,3,3	0.76	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	509/522 (97%)	0.04	4 (0%) 82 80	21, 41, 56, 71	21 (4%)
2	P	4/5 (80%)	-0.01	0 100 100	31, 32, 33, 34	1 (25%)
All	All	513/527 (97%)	0.04	4 (0%) 82 80	21, 41, 56, 71	22 (4%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	912	GLY	4.9
1	A	1223	GLY	4.6
1	A	1240	GLU	2.7
1	A	911	ASN	2.3

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

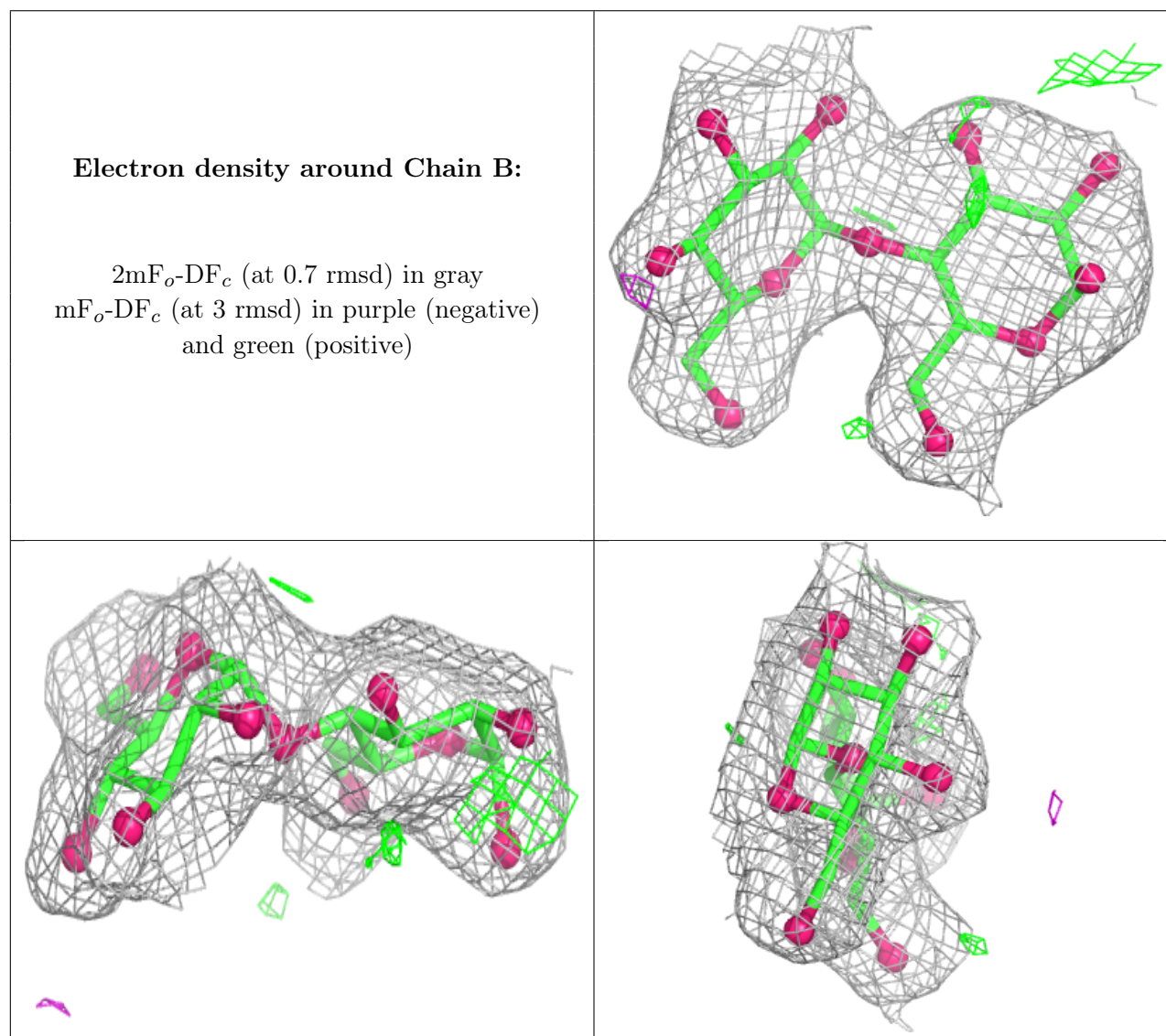
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	M3L	P	4	12/13	0.90	0.11	32,33,37,38	7

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
3	GLC	B	1	12/12	-	-	19,19,22,24	0
3	GLC	B	2	11/12	-	-	19,19,20,22	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.



6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
4	ACT	A	1	4/4	0.65	0.17	44,44,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.