



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 05:54 AM BST

PDB ID : 5LRA
Title : Plastidial phosphorylase PhoI from barley in complex with maltotetraose
Authors : Cuesta-Seijo, J.A.; Ruzanski, C.; Krucewicz, K.; Palcic, M.M.
Deposited on : 2016-08-18
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

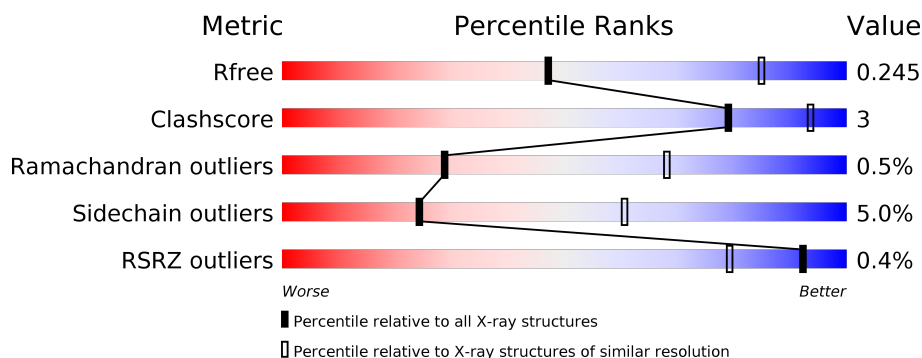
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	938	
1	B	938	
2	C	4	
2	E	4	
3	D	2	
3	F	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13697 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 Alpha-1,4 glucan phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	844	Total	C	N	O	S	0	4	1
			6740	4293	1145	1272	30			
1	B	844	Total	C	N	O	S	0	6	1
			6744	4297	1143	1273	31			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	MET	-	initiating methionine	UNP F2E0G2
A	969	THR	-	expression tag	UNP F2E0G2
A	970	PHE	-	expression tag	UNP F2E0G2
A	971	PRO	-	expression tag	UNP F2E0G2
A	972	ASP	-	expression tag	UNP F2E0G2
A	973	ILE	-	expression tag	UNP F2E0G2
A	974	GLU	-	expression tag	UNP F2E0G2
A	975	ASN	-	expression tag	UNP F2E0G2
A	976	LEU	-	expression tag	UNP F2E0G2
A	977	TYR	-	expression tag	UNP F2E0G2
A	978	PHE	-	expression tag	UNP F2E0G2
A	979	GLN	-	expression tag	UNP F2E0G2
A	980	GLY	-	expression tag	UNP F2E0G2
B	43	MET	-	initiating methionine	UNP F2E0G2
B	969	THR	-	expression tag	UNP F2E0G2
B	970	PHE	-	expression tag	UNP F2E0G2
B	971	PRO	-	expression tag	UNP F2E0G2
B	972	ASP	-	expression tag	UNP F2E0G2
B	973	ILE	-	expression tag	UNP F2E0G2
B	974	GLU	-	expression tag	UNP F2E0G2
B	975	ASN	-	expression tag	UNP F2E0G2
B	976	LEU	-	expression tag	UNP F2E0G2
B	977	TYR	-	expression tag	UNP F2E0G2
B	978	PHE	-	expression tag	UNP F2E0G2
B	979	GLN	-	expression tag	UNP F2E0G2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	980	GLY	-	expression tag	UNP F2E0G2

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



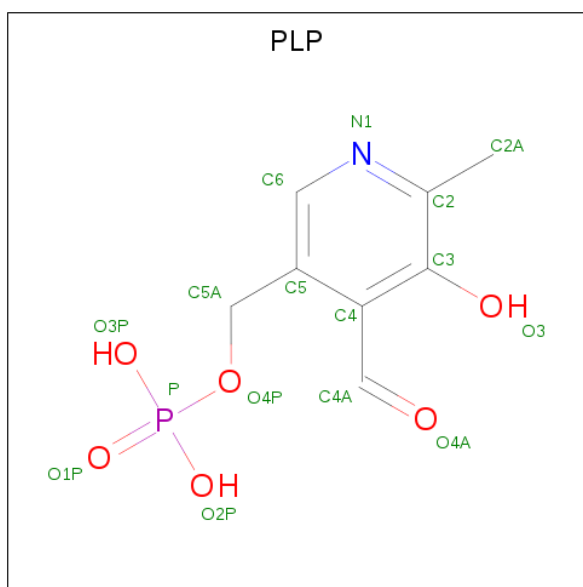
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			45	24	21			
2	E	4	Total	C	O	0	0	0
			45	24	21			

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



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

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

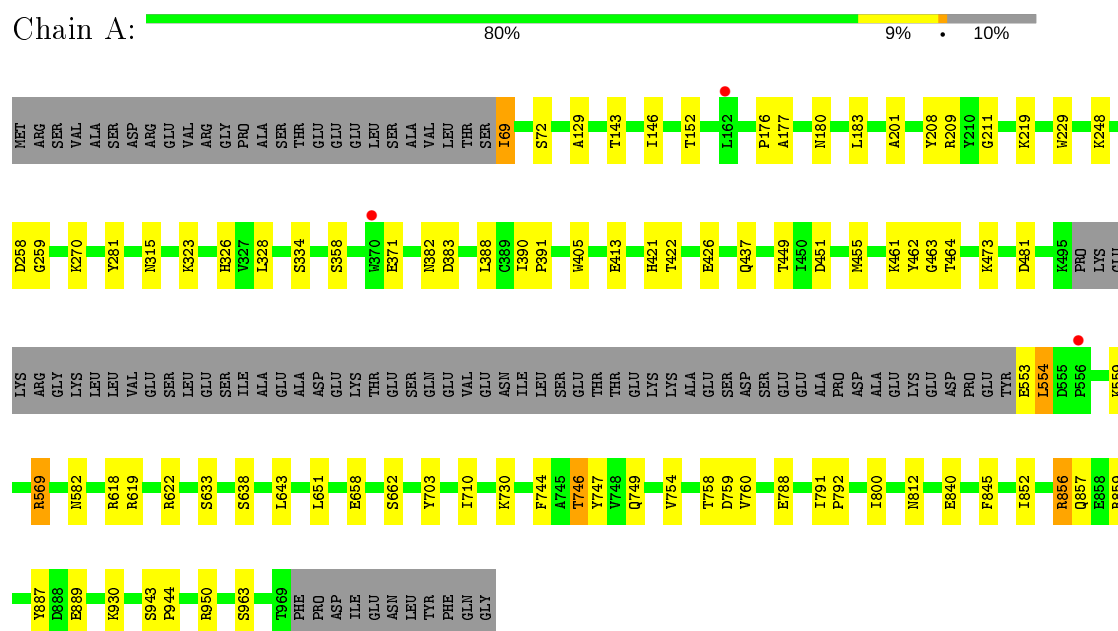
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	B	27	Total	O	0	0
			27	27		

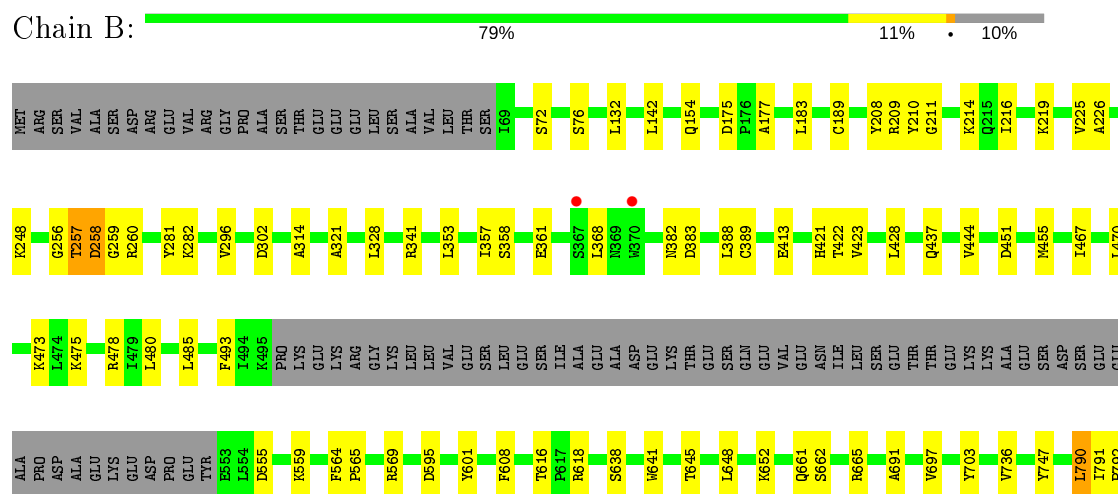
3 Residue-property plots

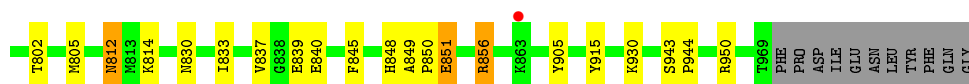
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alpha-1,4 glucan phosphorylase

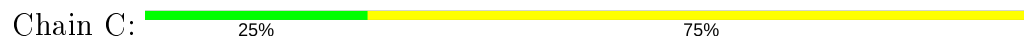


- Molecule 1: Alpha-1,4 glucan phosphorylase





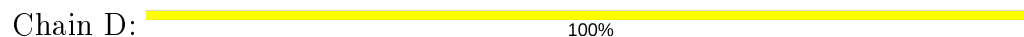
- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	227.69Å 63.15Å 148.19Å 90.00° 114.72° 90.00°	Depositor
Resolution (Å)	49.39 – 3.00 44.87 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.39-3.00) 99.9 (44.87-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.195 , 0.243 0.196 , 0.245	Depositor DCC
R_{free} test set	1165 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	73.7	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13697	wwPDB-VP
Average B, all atoms (Å ²)	91.0	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 51.41 % 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 5.6312e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.36	0/6907	0.57	0/9356
1	B	0.36	0/6917	0.57	0/9370
All	All	0.36	0/13824	0.57	0/18726

There are no bond length outliers.

There are no bond angle outliers.

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	6740	0	6632	30	0
1	B	6744	0	6637	45	0
2	C	45	0	39	0	0
2	E	45	0	39	0	0
3	D	23	0	21	0	0
3	F	23	0	21	1	0
4	A	15	0	6	0	0
4	B	15	0	6	1	0
5	A	20	0	0	2	0
5	B	27	0	0	0	0
All	All	13697	0	13401	76	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 3.

All (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:THR:O	1:B:258:ASP:HB2	1.89	0.71
1:B:848:HIS:N	1:B:851:GLU:OE1	2.32	0.59
1:A:759:ASP:OD2	1:A:887:TYR:OH	2.20	0.58
1:A:69:ILE:O	1:A:69:ILE:HG23	2.05	0.56
1:B:812:ASN:ND2	1:B:830:ASN:OD1	2.39	0.56
1:B:382:ASN:OD1	1:B:421:HIS:NE2	2.39	0.55
1:B:177:ALA:HB1	1:B:211:GLY:HA3	1.89	0.55
1:A:177:ALA:HB1	1:A:211:GLY:HA3	1.87	0.55
1:B:475:LYS:O	1:B:569:ARG:NH1	2.30	0.54
1:B:493:PHE:HB3	1:B:555:ASP:HB3	1.90	0.53
1:A:382:ASN:OD1	1:A:421:HIS:NE2	2.41	0.53
1:B:208:TYR:CE2	1:B:328:LEU:HD13	2.44	0.52
1:B:661:GLN:O	1:B:665:ARG:HG3	2.10	0.52
1:A:146:ILE:CG2	1:A:152:THR:HA	2.40	0.51
1:A:461:LYS:C	1:A:462:TYR:CD1	2.84	0.51
1:A:754:VAL:O	1:A:758:THR:HG23	2.11	0.50
1:B:943:SER:N	1:B:944:PRO:CD	2.74	0.50
1:A:143:THR:OG1	5:A:1101:HOH:O	2.20	0.49
1:A:800:ILE:HG22	1:A:845:PHE:HE1	1.77	0.49
1:B:258:ASP:O	1:B:260:ARG:HG2	2.12	0.49
1:B:132:LEU:HD22	1:B:389:CYS:SG	2.53	0.49
1:B:814:LYS:NZ	4:B:1007:PLP:O3	2.46	0.48
1:B:210:TYR:HB3	1:B:226:ALA:HB1	1.95	0.48
1:B:423:VAL:O	1:B:423:VAL:HG22	2.13	0.48
1:A:451:ASP:O	1:A:455:MET:HG3	2.13	0.47
1:A:943:SER:N	1:A:944:PRO:CD	2.77	0.47
1:B:258:ASP:C	1:B:260:ARG:N	2.67	0.47
1:B:802:THR:HB	1:B:805:MET:HG3	1.95	0.47
3:F:1:GLC:O3	3:F:2:GLC:O2	1.90	0.47
1:A:461:LYS:O	1:A:462:TYR:CD1	2.68	0.47
1:B:281:TYR:HB2	1:B:618:ARG:HD2	1.98	0.46
1:A:129:ALA:O	1:A:201:ALA:HA	2.15	0.46
1:A:749:GLN:HA	1:A:749:GLN:OE1	2.15	0.46
1:B:214:LYS:N	1:B:225:VAL:O	2.48	0.45
1:A:176:PRO:HA	1:A:229:TRP:CE3	2.51	0.45
1:B:189:CYS:SG	1:B:616:THR:HG22	2.56	0.45
1:B:302:ASP:HB3	1:B:314:ALA:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:ILE:HD11	1:A:760:VAL:HG11	1.98	0.45
1:B:849:ALA:HB3	1:B:850:PRO:HD3	1.99	0.45
1:B:353:LEU:O	1:B:357:ILE:HG12	2.16	0.44
1:A:582:ASN:ND2	5:A:1104:HOH:O	2.40	0.44
1:B:845:PHE:CE2	1:B:915:TYR:HB2	2.53	0.44
1:A:323:LYS:HA	1:A:326:HIS:CG	2.53	0.44
1:B:361:GLU:HG2	1:B:368:LEU:HD11	2.00	0.44
1:B:451:ASP:O	1:B:455:MET:HG3	2.18	0.44
1:B:258:ASP:O	1:B:260:ARG:N	2.51	0.43
1:B:691:ALA:HB3	1:B:736:VAL:HG23	2.01	0.43
1:B:833:ILE:O	1:B:837:VAL:HG22	2.18	0.43
1:B:281:TYR:CE2	1:B:282:LYS:HG3	2.54	0.43
1:A:208:TYR:CE2	1:A:328:LEU:HD13	2.52	0.43
1:B:564:PHE:HB3	1:B:565:PRO:HD2	2.00	0.43
1:B:641:TRP:O	1:B:645:THR:HA	2.19	0.43
1:B:791:ILE:HB	1:B:792:PRO:HD3	1.99	0.43
1:B:467:ILE:O	1:B:470:LEU:N	2.51	0.43
1:A:856:ARG:O	1:A:859:ARG:HB3	2.19	0.42
1:A:791:ILE:HB	1:A:792:PRO:HD3	2.01	0.42
1:A:943:SER:N	1:A:944:PRO:HD3	2.35	0.42
1:B:256:GLY:O	1:B:257:THR:C	2.58	0.42
1:B:601:TYR:HA	1:B:608:PHE:CE1	2.55	0.42
1:A:463:GLY:O	1:A:464:THR:OG1	2.30	0.41
1:A:390:ILE:HB	1:A:391:PRO:CD	2.50	0.41
1:A:481:ASP:HB2	1:A:569:ARG:CD	2.51	0.41
1:B:437:GLN:HG2	1:B:444:VAL:HG11	2.03	0.41
1:B:421:HIS:O	1:B:422:THR:HG23	2.21	0.41
1:A:619:ARG:NH1	1:A:788:GLU:OE2	2.44	0.41
1:B:943:SER:O	1:B:944:PRO:C	2.59	0.41
1:A:744:PHE:CD2	1:A:746:THR:HG22	2.56	0.41
1:B:296:VAL:HG13	1:B:321:ALA:HB2	2.03	0.41
1:B:648:LEU:HB2	1:B:944:PRO:HG3	2.02	0.41
1:A:800:ILE:HG22	1:A:845:PHE:CE1	2.56	0.41
1:B:478:ARG:HD2	1:B:480:LEU:O	2.21	0.40
1:B:697:VAL:HG11	1:B:790:LEU:HD23	2.02	0.40
1:A:281:TYR:HB2	1:A:618:ARG:HD2	2.03	0.40
1:B:856:ARG:NH1	1:B:905:TYR:O	2.51	0.40
1:A:405:TRP:CH2	1:A:449:THR:HB	2.57	0.40
1:B:455:MET:CE	1:B:485:LEU:HD22	2.50	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	844/938 (90%)	803 (95%)	37 (4%)	4 (0%)	29	68
1	B	846/938 (90%)	801 (95%)	41 (5%)	4 (0%)	29	68
All	All	1690/1876 (90%)	1604 (95%)	78 (5%)	8 (0%)	29	68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	GLY
1	B	258	ASP
1	B	259	GLY
1	A	852	ILE
1	A	258	ASP
1	A	554	LEU
1	B	142	LEU
1	B	257	THR

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	729/810 (90%)	686 (94%)	43 (6%)	19	54
1	B	730/810 (90%)	699 (96%)	31 (4%)	30	66
All	All	1459/1620 (90%)	1385 (95%)	74 (5%)	24	60

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ILE
1	A	72	SER
1	A	180	ASN
1	A	183	LEU
1	A	209	ARG
1	A	219	LYS
1	A	248	LYS
1	A	270	LYS
1	A	315	ASN
1	A	334	SER
1	A	358	SER
1	A	371	GLU
1	A	383	ASP
1	A	388	LEU
1	A	413	GLU
1	A	422	THR
1	A	426	GLU
1	A	437	GLN
1	A	473	LYS
1	A	553	GLU
1	A	554	LEU
1	A	559	LYS
1	A	569	ARG
1	A	622	ARG
1	A	633	SER
1	A	638	SER
1	A	643	LEU
1	A	651	LEU
1	A	658	GLU
1	A	662	SER
1	A	703	TYR
1	A	730	LYS
1	A	746	THR
1	A	747	TYR
1	A	812	ASN
1	A	840	GLU
1	A	856	ARG
1	A	857	GLN
1	A	889[A]	GLU
1	A	889[B]	GLU
1	A	930	LYS
1	A	950	ARG
1	A	963	SER

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Mol	Chain	Res	Type
1	B	72	SER
1	B	76	SER
1	B	154	GLN
1	B	175	ASP
1	B	183	LEU
1	B	209	ARG
1	B	216	ILE
1	B	219	LYS
1	B	248	LYS
1	B	341	ARG
1	B	358	SER
1	B	383	ASP
1	B	388	LEU
1	B	413	GLU
1	B	428	LEU
1	B	473	LYS
1	B	559	LYS
1	B	595	ASP
1	B	638	SER
1	B	652	LYS
1	B	662	SER
1	B	703	TYR
1	B	747	TYR
1	B	790	LEU
1	B	812	ASN
1	B	839	GLU
1	B	840	GLU
1	B	851	GLU
1	B	856	ARG
1	B	930	LYS
1	B	950	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	613	ASN
1	B	138	GLN
1	B	165	ASN
1	B	613	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	E	4	2	11,11,12	0.52	0	15,15,17	2.30	3 (20%)
2	GLC	E	2	2	11,11,12	0.74	0	15,15,17	1.58	2 (13%)
3	GLC	F	2	3	11,11,12	0.64	0	15,15,17	1.65	2 (13%)
2	GLC	C	2	2	11,11,12	0.59	0	15,15,17	1.57	2 (13%)
3	GLC	D	2	3	11,11,12	0.63	0	15,15,17	2.18	3 (20%)
3	GLC	F	1	3	12,12,12	0.50	0	17,17,17	0.79	0
3	GLC	D	1	3	12,12,12	0.53	0	17,17,17	3.02	5 (29%)
2	GLC	C	3	2	11,11,12	0.61	0	15,15,17	1.74	2 (13%)
2	GLC	E	3	2	11,11,12	0.74	0	15,15,17	1.18	2 (13%)
2	GLC	C	4	2	11,11,12	0.52	0	15,15,17	1.16	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	E	4	2	-	2/2/19/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
3	GLC	F	2	3	-	2/2/19/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
3	GLC	D	2	3	-	2/2/19/22	0/1/1/1
3	GLC	F	1	3	-	1/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	D	1	3	-	0/2/22/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	GLC	O1-C1-O5	8.92	137.16	110.38
2	E	4	GLC	C1-O5-C5	6.88	121.51	112.19
3	D	1	GLC	O5-C1-C2	-6.69	98.34	110.28
2	C	3	GLC	C1-O5-C5	5.84	120.11	112.19
3	D	2	GLC	C1-C2-C3	5.45	116.36	109.67
3	D	2	GLC	C1-O5-C5	5.41	119.53	112.19
2	E	2	GLC	C1-O5-C5	4.84	118.75	112.19
2	C	2	GLC	C1-O5-C5	4.53	118.32	112.19
3	F	2	GLC	C1-C2-C3	4.14	114.76	109.67
3	F	2	GLC	C1-O5-C5	4.00	117.61	112.19
2	E	4	GLC	O5-C5-C6	3.56	112.79	107.20
2	E	4	GLC	C1-C2-C3	3.53	114.00	109.67
2	C	4	GLC	C1-O5-C5	3.43	116.84	112.19
3	D	1	GLC	O1-C1-C2	-3.34	99.63	109.03
2	E	3	GLC	C1-O5-C5	2.67	115.80	112.19
3	D	2	GLC	O5-C1-C2	2.65	114.86	110.77
3	D	1	GLC	C4-C3-C2	2.44	115.08	110.82
2	C	2	GLC	O5-C5-C6	2.41	110.98	107.20
2	E	2	GLC	C1-C2-C3	2.34	112.54	109.67
3	D	1	GLC	C3-C4-C5	2.32	114.37	110.24
2	E	3	GLC	O5-C1-C2	-2.20	107.37	110.77
2	C	3	GLC	C2-C3-C4	-2.11	107.24	110.89

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	GLC	C4-C5-C6-O6
3	F	2	GLC	C4-C5-C6-O6
3	D	2	GLC	O5-C5-C6-O6
3	D	2	GLC	C4-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	E	2	GLC	O5-C5-C6-O6
3	F	2	GLC	O5-C5-C6-O6
2	E	4	GLC	O5-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	C	4	GLC	C4-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6
3	F	1	GLC	O5-C5-C6-O6
2	E	4	GLC	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

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

5.5 Carbohydrates

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BGC	C	1	2	12,12,12	0.58	0	17,17,17	0.74	0
2	GLC	C	2	2	11,11,12	0.59	0	15,15,17	1.57	2 (13%)
2	GLC	C	3	2	11,11,12	0.61	0	15,15,17	1.74	2 (13%)
2	GLC	C	4	2	11,11,12	0.52	0	15,15,17	1.16	1 (6%)
3	GLC	D	1	3	12,12,12	0.53	0	17,17,17	3.02	5 (29%)
3	GLC	D	2	3	11,11,12	0.63	0	15,15,17	2.18	3 (20%)
2	BGC	E	1	2	12,12,12	0.60	0	17,17,17	0.65	0
2	GLC	E	2	2	11,11,12	0.74	0	15,15,17	1.58	2 (13%)
2	GLC	E	3	2	11,11,12	0.74	0	15,15,17	1.18	2 (13%)
2	GLC	E	4	2	11,11,12	0.52	0	15,15,17	2.30	3 (20%)
3	GLC	F	1	3	12,12,12	0.50	0	17,17,17	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	F	2	3	11,11,12	0.64	0	15,15,17	1.65	2 (13%)

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	BGC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	2/2/19/22	0/1/1/1
3	GLC	D	1	3	-	0/2/22/22	0/1/1/1
3	GLC	D	2	3	-	2/2/19/22	0/1/1/1
2	BGC	E	1	2	-	1/2/22/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	0/1/1/1
2	GLC	E	4	2	-	2/2/19/22	0/1/1/1
3	GLC	F	1	3	-	1/2/22/22	0/1/1/1
3	GLC	F	2	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	GLC	O1-C1-O5	8.92	137.16	110.38
2	E	4	GLC	C1-O5-C5	6.88	121.51	112.19
3	D	1	GLC	O5-C1-C2	-6.69	98.34	110.28
2	C	3	GLC	C1-O5-C5	5.84	120.11	112.19
3	D	2	GLC	C1-C2-C3	5.45	116.36	109.67
3	D	2	GLC	C1-O5-C5	5.41	119.53	112.19
2	E	2	GLC	C1-O5-C5	4.84	118.75	112.19
2	C	2	GLC	C1-O5-C5	4.53	118.32	112.19
3	F	2	GLC	C1-C2-C3	4.14	114.76	109.67
3	F	2	GLC	C1-O5-C5	4.00	117.61	112.19
2	E	4	GLC	O5-C5-C6	3.56	112.79	107.20
2	E	4	GLC	C1-C2-C3	3.53	114.00	109.67
2	C	4	GLC	C1-O5-C5	3.43	116.84	112.19
3	D	1	GLC	O1-C1-C2	-3.34	99.63	109.03
2	E	3	GLC	C1-O5-C5	2.67	115.80	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	GLC	O5-C1-C2	2.65	114.86	110.77
3	D	1	GLC	C4-C3-C2	2.44	115.08	110.82
2	C	2	GLC	O5-C5-C6	2.41	110.98	107.20
2	E	2	GLC	C1-C2-C3	2.34	112.54	109.67
3	D	1	GLC	C3-C4-C5	2.32	114.37	110.24
2	E	3	GLC	O5-C1-C2	-2.20	107.37	110.77
2	C	3	GLC	C2-C3-C4	-2.11	107.24	110.89

There are no chirality outliers.

All (14) torsion outliers are listed below:

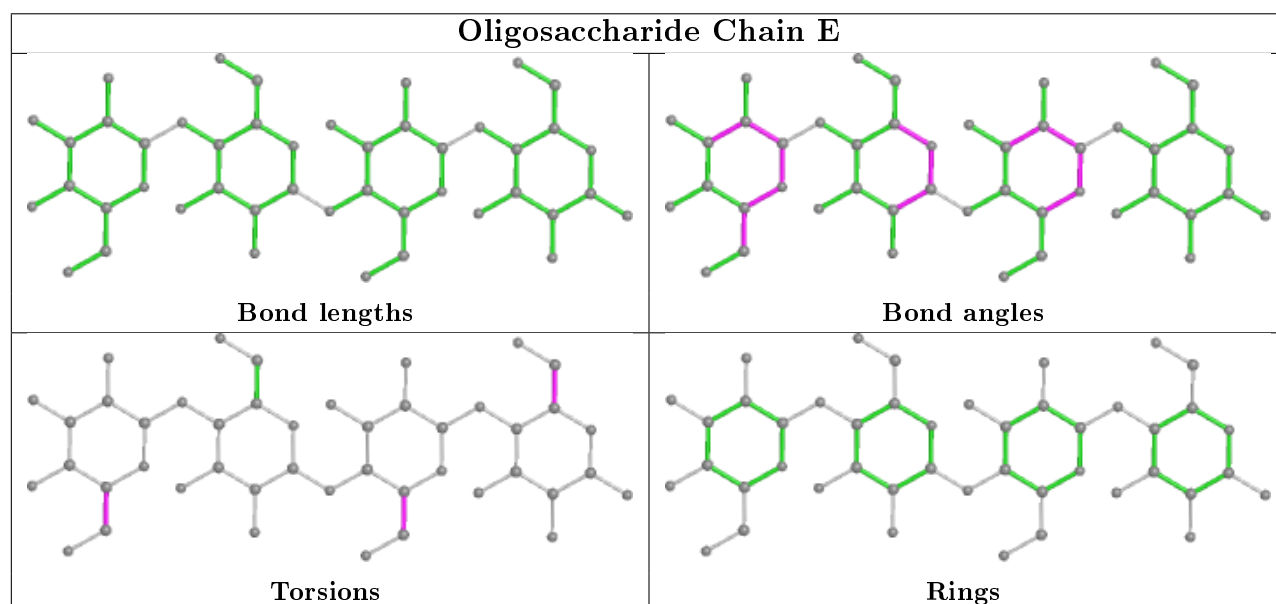
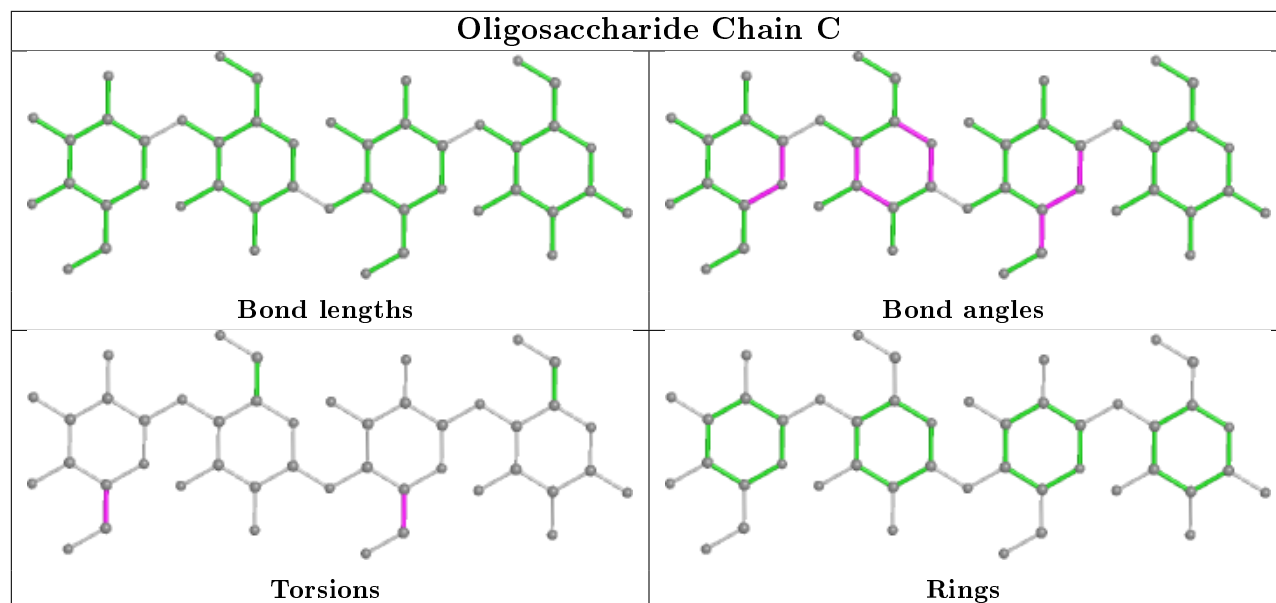
Mol	Chain	Res	Type	Atoms
2	E	2	GLC	C4-C5-C6-O6
3	F	2	GLC	C4-C5-C6-O6
3	D	2	GLC	O5-C5-C6-O6
3	D	2	GLC	C4-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6
3	F	2	GLC	O5-C5-C6-O6
2	E	4	GLC	O5-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	C	4	GLC	C4-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6
3	F	1	GLC	O5-C5-C6-O6
2	E	1	BGC	O5-C5-C6-O6
2	E	4	GLC	C4-C5-C6-O6

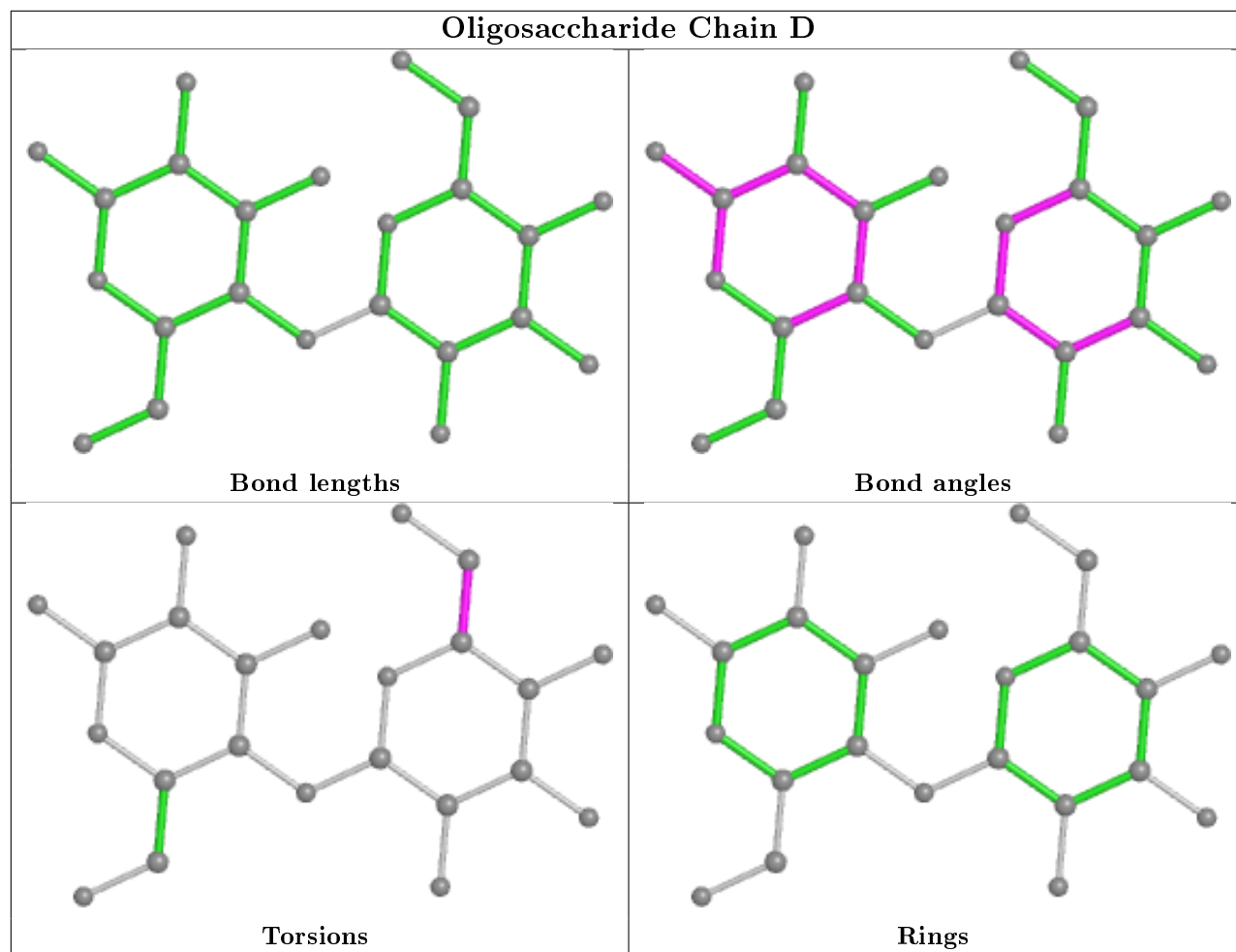
There are no ring outliers.

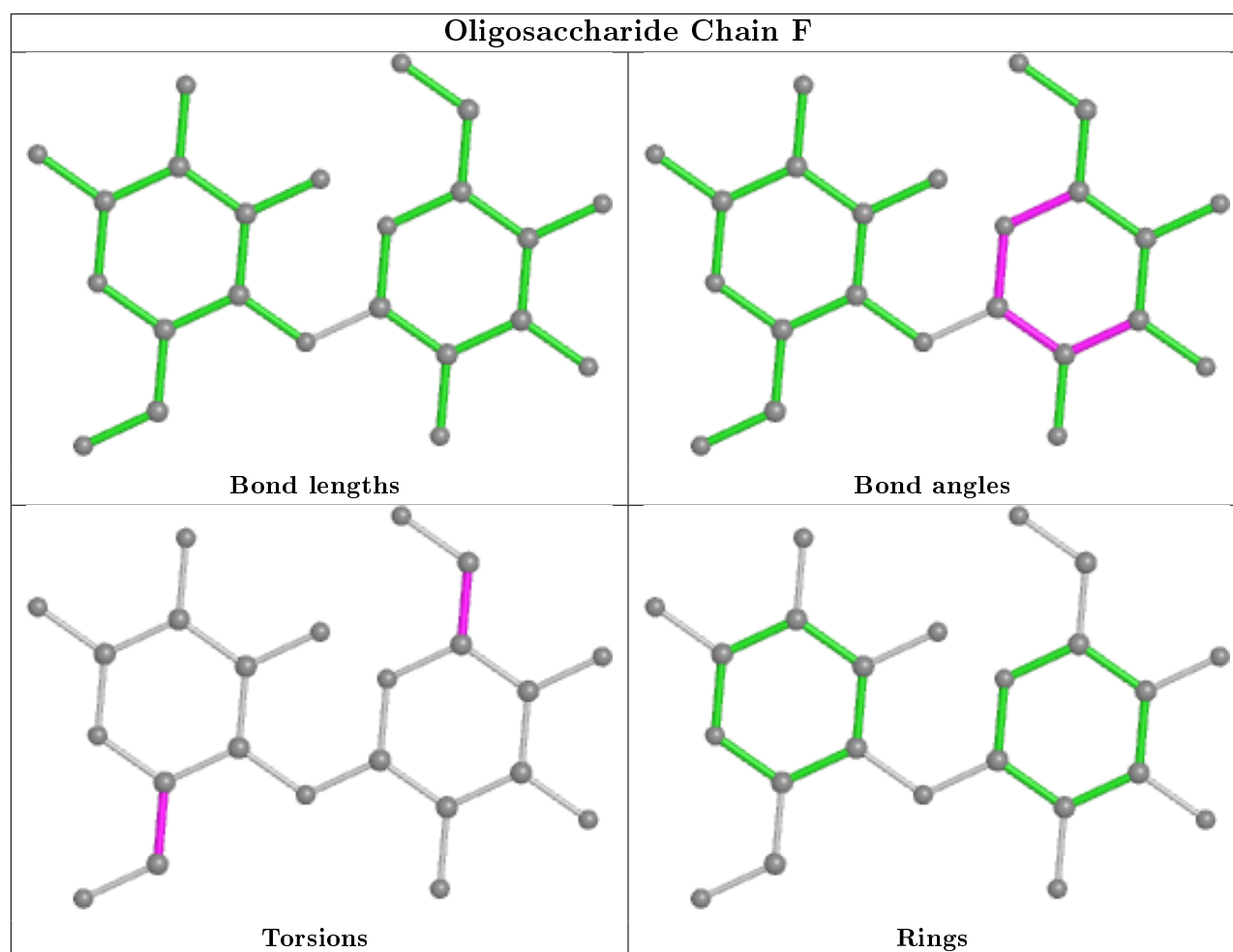
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	GLC	1	0
3	F	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](#)

2 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	PLP	B	1007	1	15,15,16	3.01	3 (20%)	20,22,23	1.23	3 (15%)
4	PLP	A	1007	1	15,15,16	2.76	3 (20%)	20,22,23	1.48	4 (20%)

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	PLP	B	1007	1	-	3/6/6/8	0/1/1/1
4	PLP	A	1007	1	-	4/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1007	PLP	C3-C2	7.87	1.48	1.40
4	A	1007	PLP	C5-C4	7.79	1.49	1.40
4	B	1007	PLP	C5-C4	7.31	1.48	1.40
4	A	1007	PLP	C3-C2	5.71	1.46	1.40
4	B	1007	PLP	C3-C4	3.63	1.47	1.40
4	A	1007	PLP	C3-C4	3.55	1.47	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1007	PLP	C4A-C4-C5	3.19	124.22	120.94
4	A	1007	PLP	C2A-C2-C3	-2.71	117.54	120.89
4	B	1007	PLP	O3-C3-C2	2.26	122.41	117.49
4	B	1007	PLP	C4A-C4-C5	2.25	123.25	120.94
4	A	1007	PLP	C2A-C2-N1	2.13	121.82	117.67
4	A	1007	PLP	C6-N1-C2	2.08	123.01	119.17
4	B	1007	PLP	C6-N1-C2	2.03	122.92	119.17

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1007	PLP	C5A-O4P-P-O2P
4	A	1007	PLP	C5A-O4P-P-O2P
4	A	1007	PLP	C5A-O4P-P-O3P
4	B	1007	PLP	C5A-O4P-P-O1P
4	B	1007	PLP	C5A-O4P-P-O3P
4	A	1007	PLP	C5A-O4P-P-O1P
4	A	1007	PLP	C4-C5-C5A-O4P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1007	PLP	1	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	844/938 (89%)	-0.37	3 (0%) 92 79	56, 88, 127, 172	0
1	B	844/938 (89%)	-0.34	3 (0%) 92 79	46, 89, 129, 170	0
All	All	1688/1876 (89%)	-0.35	6 (0%) 92 79	46, 88, 129, 172	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	370	TRP	3.7
1	A	370	TRP	2.5
1	A	556	PRO	2.3
1	B	367	SER	2.3
1	B	863	LYS	2.2
1	A	162	LEU	2.0

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

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	F	2	11/12	0.73	0.33	121,130,142,143	0
3	GLC	F	1	12/12	0.77	0.36	146,158,162,164	0
3	GLC	D	2	11/12	0.79	0.30	116,129,136,137	0
3	GLC	D	1	12/12	0.80	0.34	124,135,141,144	0
2	GLC	C	4	11/12	0.90	0.34	77,89,99,99	0
2	GLC	E	4	11/12	0.92	0.28	76,82,87,93	0
2	GLC	C	2	11/12	0.92	0.20	86,90,96,97	0
2	GLC	E	2	11/12	0.94	0.16	68,75,81,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	E	3	11/12	0.97	0.23	72,74,78,81	0
2	GLC	C	3	11/12	0.98	0.25	86,88,90,90	0

6.3 Carbohydrates

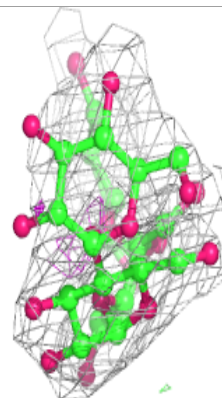
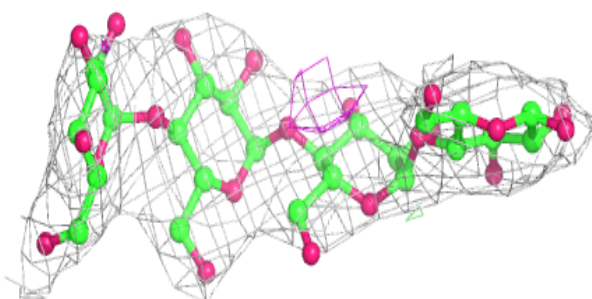
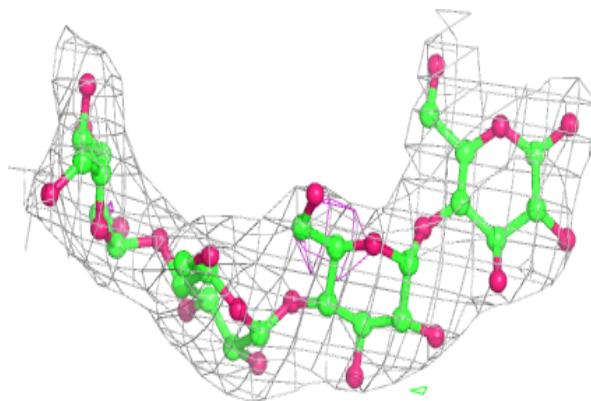
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GLC	F	2	11/12	0.73	0.33	121,130,142,143	0
3	GLC	F	1	12/12	0.77	0.36	146,158,162,164	0
3	GLC	D	2	11/12	0.79	0.30	116,129,136,137	0
3	GLC	D	1	12/12	0.80	0.34	124,135,141,144	0
2	GLC	C	4	11/12	0.90	0.34	77,89,99,99	0
2	BGC	E	1	12/12	0.91	0.17	89,96,105,110	0
2	GLC	C	2	11/12	0.92	0.20	86,90,96,97	0
2	GLC	E	4	11/12	0.92	0.28	76,82,87,93	0
2	BGC	C	1	12/12	0.93	0.15	96,101,104,107	0
2	GLC	E	2	11/12	0.94	0.16	68,75,81,82	0
2	GLC	E	3	11/12	0.97	0.23	72,74,78,81	0
2	GLC	C	3	11/12	0.98	0.25	86,88,90,90	0

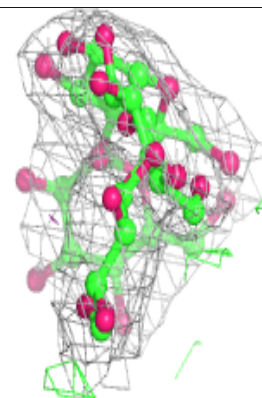
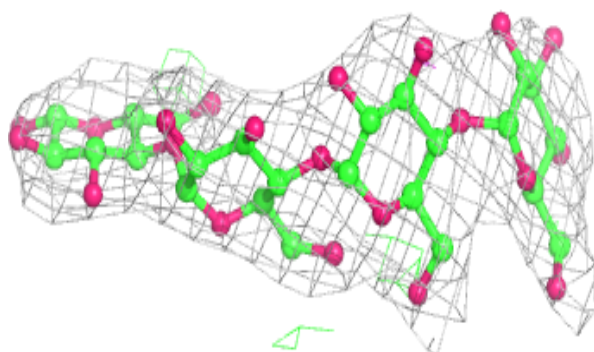
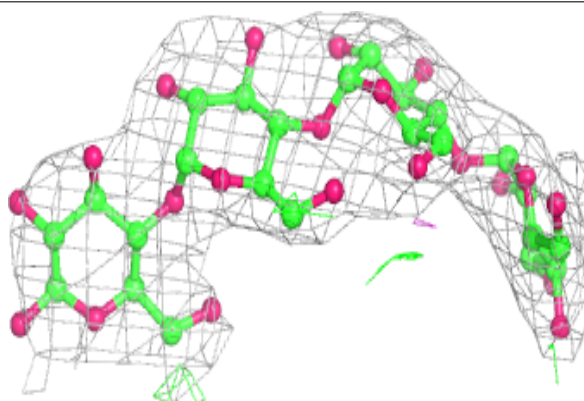
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

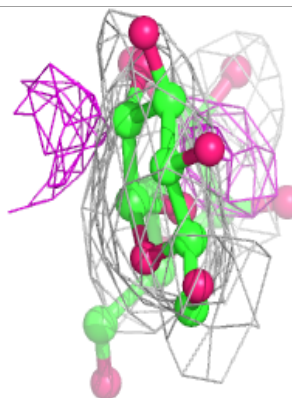
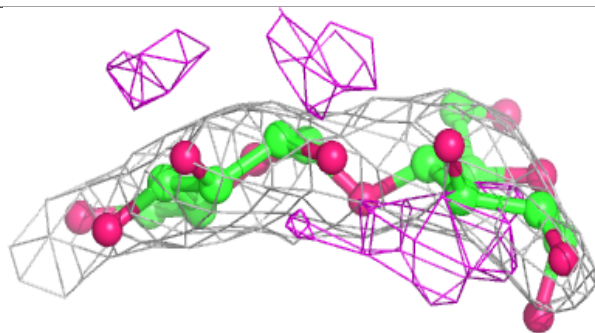
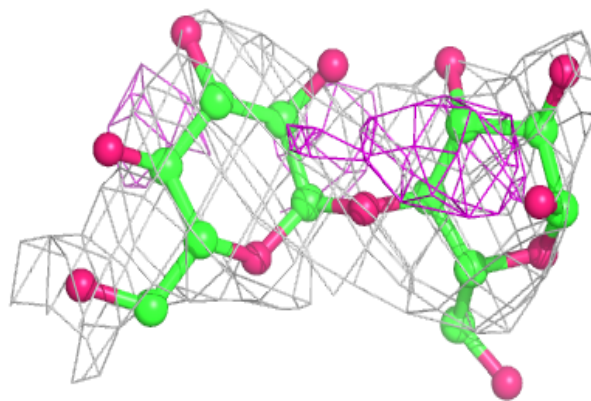
**Electron density around Chain E:**

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

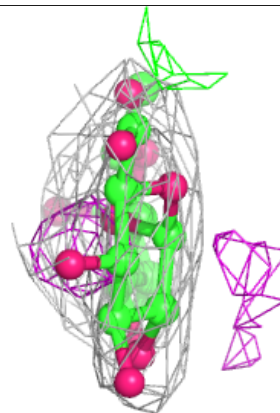
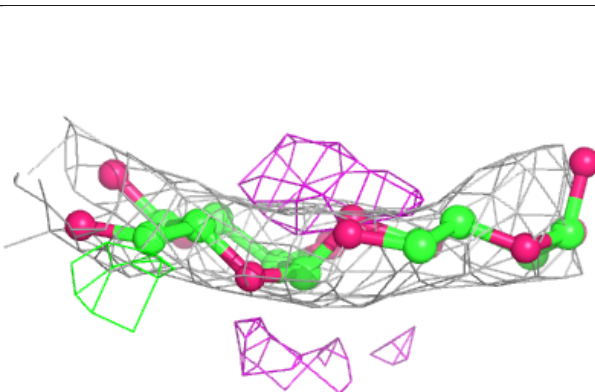
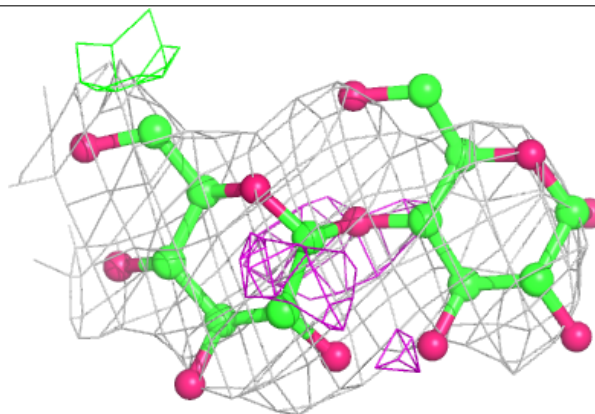


Electron density around Chain D:

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

**Electron density around Chain F:**

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
4	PLP	A	1007	15/16	0.96	0.26	61,67,75,76	0
4	PLP	B	1007	15/16	0.97	0.26	55,61,70,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.