WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 04:59 PM JST

PDB ID	:	5ZQX
Title	:	Crystal structure of beta-xylosidase mutant (E186Q) from Bacillus pumilus
Authors	:	Ha, N.C.; Hong, S.; Jo, I.
Deposited on	:	2018-04-20
Resolution	:	2.00 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 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:

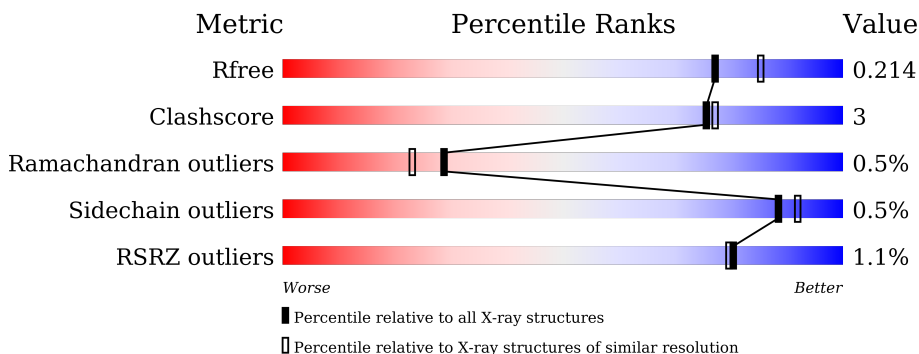|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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.
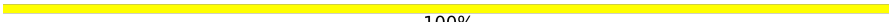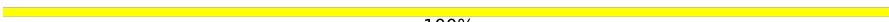
Metric	Percentile Ranks	Value
Rfree		0.214
Clashscore		3
Ramachandran outliers		0.5%
Sidechain outliers		0.5%
RSRZ outliers		1.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

❚ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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 <=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	541	% 92% 7% •
1	B	541	2% 88% 10% •
1	C	541	% 90% 9% •
1	D	541	% 91% 8% •
2	E	2	100%
2	F	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	G	2	100%
2	H	2	100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18427 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 Beta-xylosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4345	2796	729	808	12			
1	B	533	Total	C	N	O	S	0	0	0
			4319	2781	724	802	12			
1	C	535	Total	C	N	O	S	0	0	0
			4335	2790	726	807	12			
1	D	533	Total	C	N	O	S	0	0	0
			4319	2781	724	802	12			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	GLN	GLU	engineered mutation	UNP P07129
A	536	HIS	-	expression tag	UNP P07129
A	537	HIS	-	expression tag	UNP P07129
A	538	HIS	-	expression tag	UNP P07129
A	539	HIS	-	expression tag	UNP P07129
A	540	HIS	-	expression tag	UNP P07129
A	541	HIS	-	expression tag	UNP P07129
B	186	GLN	GLU	engineered mutation	UNP P07129
B	536	HIS	-	expression tag	UNP P07129
B	537	HIS	-	expression tag	UNP P07129
B	538	HIS	-	expression tag	UNP P07129
B	539	HIS	-	expression tag	UNP P07129
B	540	HIS	-	expression tag	UNP P07129
B	541	HIS	-	expression tag	UNP P07129
C	186	GLN	GLU	engineered mutation	UNP P07129
C	536	HIS	-	expression tag	UNP P07129
C	537	HIS	-	expression tag	UNP P07129
C	538	HIS	-	expression tag	UNP P07129
C	539	HIS	-	expression tag	UNP P07129
C	540	HIS	-	expression tag	UNP P07129
C	541	HIS	-	expression tag	UNP P07129

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Chain	Residue	Modelled	Actual	Comment	Reference
D	186	GLN	GLU	engineered mutation	UNP P07129
D	536	HIS	-	expression tag	UNP P07129
D	537	HIS	-	expression tag	UNP P07129
D	538	HIS	-	expression tag	UNP P07129
D	539	HIS	-	expression tag	UNP P07129
D	540	HIS	-	expression tag	UNP P07129
D	541	HIS	-	expression tag	UNP P07129

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total 19	C 10	O 9	0	0	0
2	F	2	Total 19	C 10	O 9	0	0	0
2	G	2	Total 19	C 10	O 9	0	0	0
2	H	2	Total 19	C 10	O 9	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	254	Total 254	O 254	0	0
3	B	227	Total 227	O 227	0	0
3	C	276	Total 276	O 276	0	0
3	D	276	Total 276	O 276	0	0

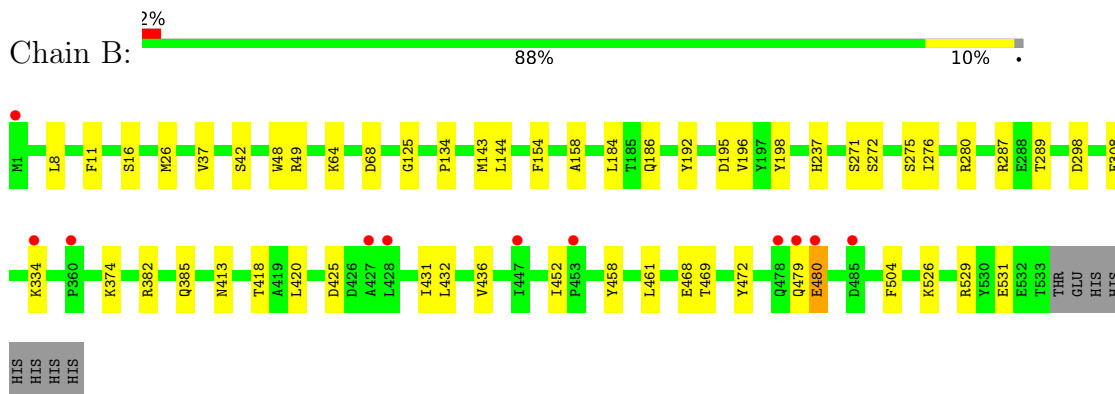# 3 Residue-property plots ⓘ

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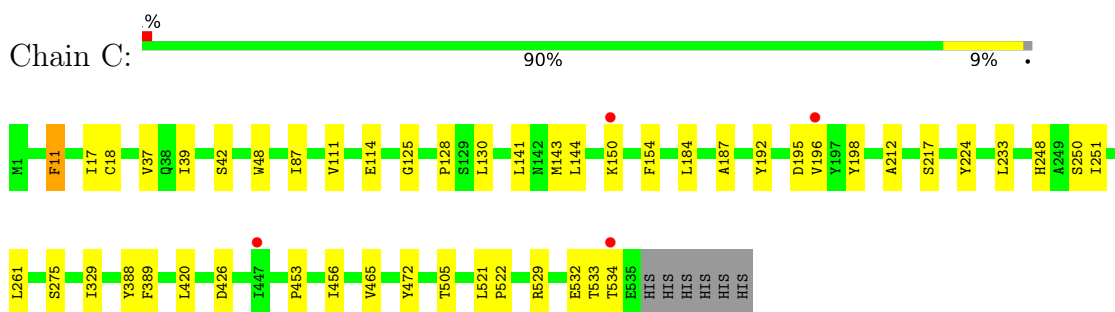
- Molecule 1: Beta-xylosidase
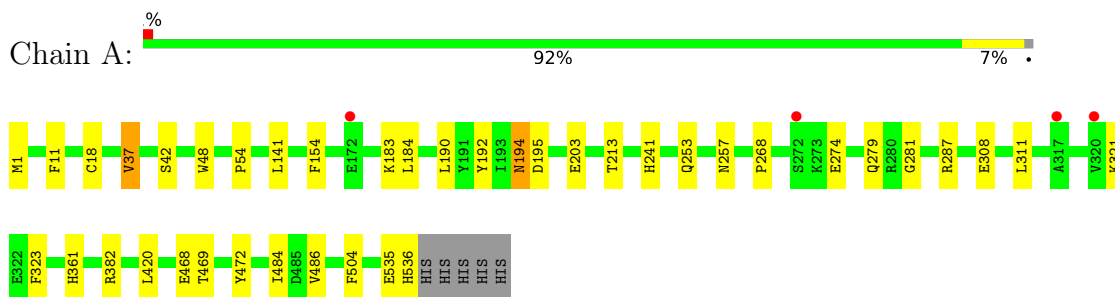
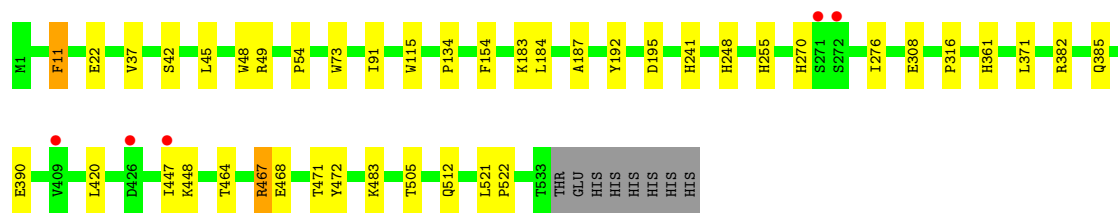
- Molecule 1: Beta-xylosidase

- Molecule 1: Beta-xylosidase

- Molecule 1: Beta-xylosidase

M1 F11 E22 V37 S42 L45 W48 R49 P54 W73 I91 W115 P134 F154 K183 L184 A187 Y192 D195 H241 H248 H255 H270 S271 S272 I276 E308 P316 H361 L371 R382 Q385

E390 V409 L420 D426 I447 K448 T464 R467 E468 T471 Y472 K483 T505 Q512 L521 P522 T533 THR GLU HIS HIS HIS HIS HIS HIS

• Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain E:

100%

XYP1 XYP2

• Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose
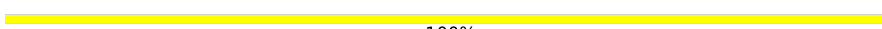
Chain F:

50%   50%

XYP1 XYP2

• Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain G:

100%

XYP1 XYP2

• Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain H:

100%

XYP1 XYP2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.26Å 104.78Å 113.16Å 90.00° 111.13° 90.00°	Depositor
Resolution (Å)	30.70 – 2.00 30.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.6 (30.70-2.00) 89.6 (30.70-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.94 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.11.1-2575)	Depositor
R, R_{free}	0.170 , 0.214 0.170 , 0.214	Depositor DCC
R_{free} test set	6799 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.4	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18427	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4351e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: XYP

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	0.28	0/4482	0.50	0/6097
1	B	0.27	0/4455	0.50	0/6060
1	C	0.28	0/4471	0.50	0/6082
1	D	0.28	0/4455	0.51	0/6060
All	All	0.28	0/17863	0.50	0/24299

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	4345	0	4156	21	0
1	B	4319	0	4136	31	0
1	C	4335	0	4149	26	0
1	D	4319	0	4136	29	0
2	E	19	0	0	0	0
2	F	19	0	0	1	0
2	G	19	0	0	0	0
2	H	19	0	0	0	0
3	A	254	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	227	0	0	3	0
3	C	276	0	0	0	1
3	D	276	0	0	1	1
All	All	18427	0	16577	105	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 3.

All (105) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:ILE:HD12	1:D:448:LYS:N	1.58	1.15
1:D:447:ILE:HD12	1:D:448:LYS:H	1.25	0.98
1:D:447:ILE:CD1	1:D:448:LYS:N	2.45	0.76
1:D:471:THR:HG21	1:D:483:LYS:HE2	1.77	0.67
1:D:447:ILE:CD1	1:D:448:LYS:HB2	2.26	0.66
1:B:382:ARG:NH2	1:B:385:GLN:OE1	2.31	0.64
1:B:275:SER:HB2	1:D:183:LYS:HB2	1.80	0.62
1:A:192:TYR:CZ	1:A:195:ASP:HA	2.35	0.61
1:C:453:PRO:HG2	1:C:456:ILE:HG12	1.83	0.60
1:D:467:ARG:HB3	1:D:468:GLU:OE1	2.02	0.60
1:C:39:ILE:HG21	1:C:111:VAL:HG21	1.83	0.59
1:C:196:VAL:HG13	1:C:198:TYR:CE1	2.38	0.59
1:D:390:GLU:HG2	1:D:464:THR:HG23	1.87	0.56
1:B:42:SER:HB2	1:B:48:TRP:CD2	2.41	0.56
1:B:468:GLU:HG2	1:B:469:THR:HG23	1.89	0.54
1:B:529:ARG:NH1	1:B:531:GLU:OE1	2.40	0.54
1:A:194:ASN:O	1:A:194:ASN:ND2	2.40	0.54
1:D:468:GLU:OE1	1:D:468:GLU:N	2.39	0.54
1:B:420:LEU:HD22	1:B:472:TYR:HB3	1.91	0.53
1:C:192:TYR:CZ	1:C:195:ASP:HA	2.44	0.52
1:D:382:ARG:NH2	1:D:385:GLN:OE1	2.42	0.52
1:D:192:TYR:CZ	1:D:195:ASP:HA	2.46	0.51
1:D:447:ILE:HD12	1:D:448:LYS:CB	2.41	0.50
1:A:361:HIS:O	3:A:701:HOH:O	2.20	0.50
1:A:253:GLN:NE2	1:A:257:ASN:OD1	2.45	0.49
1:D:447:ILE:HD12	1:D:448:LYS:CA	2.41	0.49
1:D:134:PRO:HG3	1:D:192:TYR:CD2	2.48	0.48
1:A:268:PRO:HB2	1:A:281:GLY:HA3	1.96	0.48
1:B:154:PHE:CG	1:B:184:LEU:HA	2.49	0.48
1:C:420:LEU:HD22	1:C:472:TYR:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ILE:HG12	1:C:261:LEU:HD12	1.96	0.48
1:D:382:ARG:HD2	3:D:929:HOH:O	2.13	0.48
1:B:192:TYR:CZ	1:B:195:ASP:HA	2.49	0.47
1:A:183:LYS:HB2	1:C:275:SER:HB2	1.96	0.47
1:B:432:LEU:HB2	1:B:452:ILE:HD11	1.96	0.47
1:D:420:LEU:HD22	1:D:472:TYR:HB3	1.95	0.47
1:A:468:GLU:HG2	1:A:469:THR:HG23	1.97	0.47
1:B:134:PRO:HG3	1:B:192:TYR:CD2	2.49	0.47
1:A:535:GLU:O	1:A:536:HIS:HB2	2.14	0.47
1:A:141:LEU:HD11	1:A:190:LEU:HD12	1.97	0.46
1:D:54:PRO:HB3	1:D:115:TRP:CD1	2.51	0.46
1:B:125:GLY:HA3	1:B:143:MET:O	2.16	0.46
1:B:196:VAL:HG23	1:B:198:TYR:CE1	2.50	0.46
1:B:271:SER:O	1:B:272:SER:HB3	2.16	0.46
1:D:22:GLU:HG2	1:D:255:HIS:CG	2.51	0.46
1:A:484:ILE:HG22	1:A:486:VAL:HG12	1.98	0.45
1:C:87:ILE:HD11	1:C:130:LEU:CB	2.47	0.45
1:B:418:THR:HG22	1:B:436:VAL:HG13	1.99	0.45
1:A:203:GLU:OE1	1:A:213:THR:HG21	2.16	0.45
1:B:42:SER:HB2	1:B:48:TRP:CE3	2.52	0.45
1:B:479:GLN:O	1:B:480:GLU:HB2	2.17	0.45
1:C:42:SER:HB2	1:C:48:TRP:CD2	2.52	0.45
1:C:154:PHE:CG	1:C:184:LEU:HA	2.51	0.45
1:A:154:PHE:CG	1:A:184:LEU:HA	2.52	0.45
1:B:374:LYS:NZ	3:B:705:HOH:O	2.43	0.45
1:C:388:TYR:HB3	1:C:533:THR:HG23	1.99	0.45
1:A:1:MET:HB3	1:A:1:MET:HE2	1.90	0.44
1:D:154:PHE:CG	1:D:184:LEU:HA	2.52	0.44
1:B:186:GLN:NE2	2:F:1:XYP:O4	2.49	0.44
1:D:241:HIS:CD2	1:D:308:GLU:HB3	2.52	0.44
1:D:521:LEU:HD12	1:D:522:PRO:HD2	1.99	0.44
1:A:420:LEU:HD22	1:A:472:TYR:HB3	1.98	0.44
1:A:311:LEU:HD12	1:A:311:LEU:HA	1.89	0.44
1:C:144:LEU:HD23	1:C:144:LEU:HA	1.89	0.44
1:D:187:ALA:HB2	1:D:248:HIS:CE1	2.53	0.44
1:B:425:ASP:HB2	1:B:431:ILE:HD13	1.99	0.44
1:B:64:LYS:NZ	3:B:708:HOH:O	2.46	0.44
1:C:87:ILE:HD11	1:C:130:LEU:HB2	2.00	0.44
1:C:187:ALA:HB2	1:C:248:HIS:CE1	2.53	0.43
1:B:16:SER:O	1:B:26:MET:HA	2.17	0.43
1:B:287:ARG:NH2	1:B:504:PHE:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:HIS:NE2	1:B:308:GLU:OE2	2.40	0.43
1:C:533:THR:HG23	1:C:533:THR:O	2.19	0.43
1:D:270:HIS:CE1	1:D:276:ILE:HD11	2.54	0.43
1:C:217:SER:HB2	1:C:224:TYR:HA	2.01	0.42
1:B:432:LEU:HD11	1:B:461:LEU:HD21	2.01	0.42
1:A:287:ARG:NH2	1:A:504:PHE:HB3	2.34	0.42
1:A:274:GLU:HG2	1:A:279:GLN:HB3	2.02	0.42
1:D:45:LEU:HD12	1:D:316:PRO:HG3	2.02	0.42
1:B:458:TYR:CE2	1:B:526:LYS:HB2	2.55	0.42
1:C:532:GLU:HB3	1:C:534:THR:HG23	2.02	0.42
1:A:42:SER:HB2	1:A:48:TRP:CD2	2.55	0.42
1:C:17:ILE:HG22	1:C:250:SER:OG	2.20	0.42
1:C:212:ALA:HB3	1:C:233:LEU:HB3	2.02	0.42
1:A:321:LYS:HE2	1:A:323:PHE:CE1	2.54	0.41
1:B:49:ARG:NH2	3:B:718:HOH:O	2.52	0.41
1:D:11:PHE:CE1	1:D:505:THR:HA	2.56	0.41
1:A:37:VAL:HB	1:A:54:PRO:HD2	2.02	0.41
1:B:68:ASP:CG	1:B:413:ASN:HB2	2.41	0.41
1:D:42:SER:HB2	1:D:48:TRP:CD2	2.55	0.41
1:C:125:GLY:HA3	1:C:143:MET:O	2.20	0.41
1:C:150:LYS:HD3	1:C:150:LYS:HA	1.76	0.41
1:D:73:TRP:CD2	1:D:91:ILE:HG13	2.56	0.41
1:A:241:HIS:CD2	1:A:308:GLU:HB3	2.56	0.41
1:C:329:ILE:O	1:C:529:ARG:HA	2.20	0.41
1:B:8:LEU:HB2	1:B:289:THR:HB	2.03	0.41
1:C:128:PRO:HA	1:C:141:LEU:O	2.21	0.41
1:D:371:LEU:HD21	1:D:512:GLN:HG3	2.03	0.41
1:D:447:ILE:CD1	1:D:448:LYS:CB	2.94	0.41
1:B:144:LEU:HD23	1:B:144:LEU:HA	1.97	0.41
1:B:144:LEU:HG	1:B:158:ALA:HB2	2.03	0.40
1:B:276:ILE:O	1:B:280:ARG:HD2	2.21	0.40
1:C:11:PHE:CE1	1:C:505:THR:HA	2.56	0.40
1:C:521:LEU:HD12	1:C:522:PRO:HD2	2.04	0.40
1:C:389:PHE:CZ	1:C:465:VAL:HG21	2.57	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)
3:C:919:HOH:O	3:D:952:HOH:O[2_555]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	534/541 (99%)	505 (95%)	27 (5%)	2 (0%)	34	30
1	B	531/541 (98%)	500 (94%)	28 (5%)	3 (1%)	25	19
1	C	533/541 (98%)	505 (95%)	26 (5%)	2 (0%)	34	30
1	D	531/541 (98%)	502 (94%)	26 (5%)	3 (1%)	25	19
All	All	2129/2164 (98%)	2012 (94%)	107 (5%)	10 (0%)	29	23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	480	GLU
1	A	11	PHE
1	A	37	VAL
1	B	37	VAL
1	C	37	VAL
1	D	37	VAL
1	B	11	PHE
1	D	11	PHE
1	C	11	PHE
1	D	467	ARG

5.3.2 Protein sidechains (i)

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	467/472 (99%)	464 (99%)	3 (1%)	86	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	464/472 (98%)	462 (100%)	2 (0%)	91	93
1	C	466/472 (99%)	463 (99%)	3 (1%)	86	90
1	D	464/472 (98%)	462 (100%)	2 (0%)	91	93
All	All	1861/1888 (99%)	1851 (100%)	10 (0%)	88	92

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	CYS
1	A	194	ASN
1	A	382	ARG
1	B	298	ASP
1	B	334	LYS
1	C	18	CYS
1	C	114	GLU
1	C	426	ASP
1	D	49	ARG
1	D	361	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	186	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	XYP	E	1	2	10,10,10	1.86	4 (40%)	14,14,14	0.95	1 (7%)
2	XYP	E	2	2	9,9,10	3.12	6 (66%)	10,12,14	2.14	2 (20%)
2	XYP	F	1	2	10,10,10	1.86	3 (30%)	14,14,14	1.06	1 (7%)
2	XYP	F	2	2	9,9,10	3.19	7 (77%)	10,12,14	2.03	3 (30%)
2	XYP	G	1	2	10,10,10	1.78	4 (40%)	14,14,14	1.03	2 (14%)
2	XYP	G	2	2	9,9,10	3.12	6 (66%)	10,12,14	1.95	3 (30%)
2	XYP	H	1	2	10,10,10	1.76	4 (40%)	14,14,14	1.04	2 (14%)
2	XYP	H	2	2	9,9,10	3.08	7 (77%)	10,12,14	2.04	3 (30%)

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	XYP	E	1	2	-	-	0/1/1/1
2	XYP	E	2	2	-	-	0/1/1/1
2	XYP	F	1	2	-	-	0/1/1/1
2	XYP	F	2	2	-	-	0/1/1/1
2	XYP	G	1	2	-	-	0/1/1/1
2	XYP	G	2	2	-	-	0/1/1/1
2	XYP	H	1	2	-	-	0/1/1/1
2	XYP	H	2	2	-	-	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	XYP	C4-C3	-6.19	1.43	1.52
2	G	2	XYP	C4-C3	-6.10	1.43	1.52
2	F	2	XYP	C4-C3	-6.07	1.43	1.52
2	H	2	XYP	C4-C3	-5.97	1.43	1.52
2	F	2	XYP	O5-C1	4.11	1.50	1.42
2	G	2	XYP	O5-C1	3.84	1.50	1.42
2	E	2	XYP	O5-C1	3.72	1.50	1.42
2	H	2	XYP	O5-C1	3.68	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	XYP	O3-C3	3.16	1.50	1.43
2	E	2	XYP	O3-C3	3.14	1.50	1.43
2	H	2	XYP	O3-C3	3.09	1.50	1.43
2	F	2	XYP	O3-C3	3.07	1.50	1.43
2	E	2	XYP	C1-C2	3.06	1.59	1.52
2	F	1	XYP	O5-C1	3.05	1.47	1.43
2	F	2	XYP	C1-C2	2.98	1.59	1.52
2	E	1	XYP	O5-C1	2.97	1.47	1.43
2	E	1	XYP	C4-C3	-2.97	1.48	1.52
2	G	1	XYP	O5-C1	2.95	1.47	1.43
2	H	1	XYP	O5-C1	2.94	1.47	1.43
2	F	1	XYP	C4-C3	-2.90	1.48	1.52
2	H	2	XYP	C1-C2	2.89	1.58	1.52
2	G	2	XYP	C1-C2	2.80	1.58	1.52
2	F	1	XYP	O5-C5	2.71	1.48	1.43
2	G	2	XYP	O5-C5	2.68	1.48	1.42
2	F	2	XYP	O5-C5	2.65	1.48	1.42
2	H	2	XYP	O5-C5	2.64	1.48	1.42
2	E	1	XYP	O5-C5	2.62	1.47	1.43
2	H	1	XYP	O5-C5	2.61	1.47	1.43
2	G	1	XYP	O5-C5	2.58	1.47	1.43
2	G	1	XYP	C4-C3	-2.49	1.48	1.52
2	F	2	XYP	O4-C4	2.48	1.48	1.43
2	G	2	XYP	O4-C4	2.48	1.48	1.43
2	H	2	XYP	O4-C4	2.47	1.48	1.43
2	E	2	XYP	O5-C5	2.46	1.47	1.42
2	F	2	XYP	C2-C3	-2.37	1.49	1.52
2	H	1	XYP	C4-C3	-2.36	1.49	1.52
2	E	2	XYP	O4-C4	2.25	1.48	1.43
2	H	2	XYP	C2-C3	-2.13	1.49	1.52
2	E	1	XYP	O3-C3	2.11	1.47	1.43
2	H	1	XYP	O3-C3	2.07	1.47	1.43
2	G	1	XYP	O3-C3	2.00	1.47	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	XYP	C1-C2-C3	5.52	116.45	109.67
2	F	2	XYP	C1-C2-C3	4.91	115.71	109.67
2	G	2	XYP	C1-C2-C3	4.67	115.40	109.67
2	H	2	XYP	C1-C2-C3	4.30	114.95	109.67
2	H	2	XYP	C4-C3-C2	3.50	115.08	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	XYP	C4-C3-C2	3.04	114.53	110.92
2	F	2	XYP	C4-C3-C2	2.87	114.33	110.92
2	G	2	XYP	C4-C3-C2	2.72	114.15	110.92
2	G	1	XYP	O4-C4-C3	2.53	115.21	110.14
2	H	2	XYP	C5-C4-C3	2.36	112.57	109.67
2	H	1	XYP	O4-C4-C3	2.32	114.78	110.14
2	G	2	XYP	C5-C4-C3	2.23	112.41	109.67
2	F	2	XYP	C5-C4-C3	2.23	112.40	109.67
2	E	1	XYP	O4-C4-C3	2.18	114.50	110.14
2	H	1	XYP	C5-C4-C3	2.09	112.24	109.67
2	G	1	XYP	C5-C4-C3	2.06	112.19	109.67
2	F	1	XYP	C5-C4-C3	2.01	112.13	109.67

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
2	F	1	XYP	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.

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings
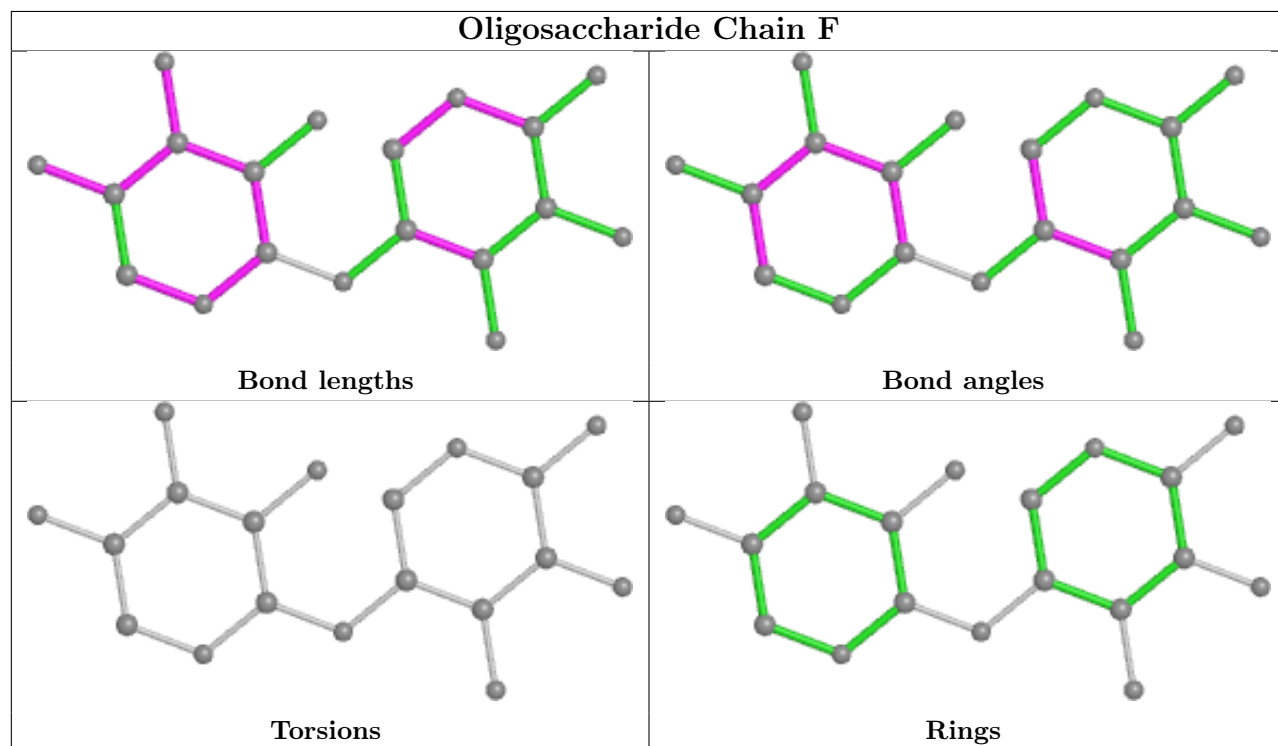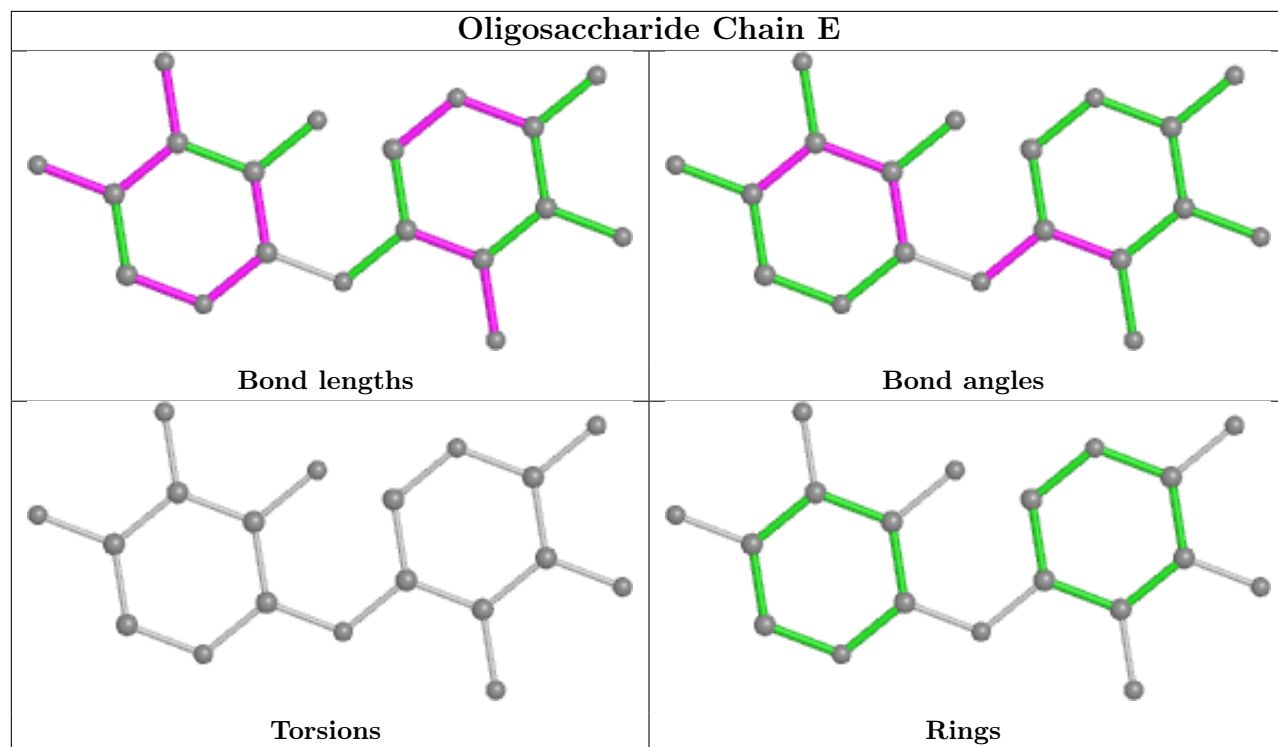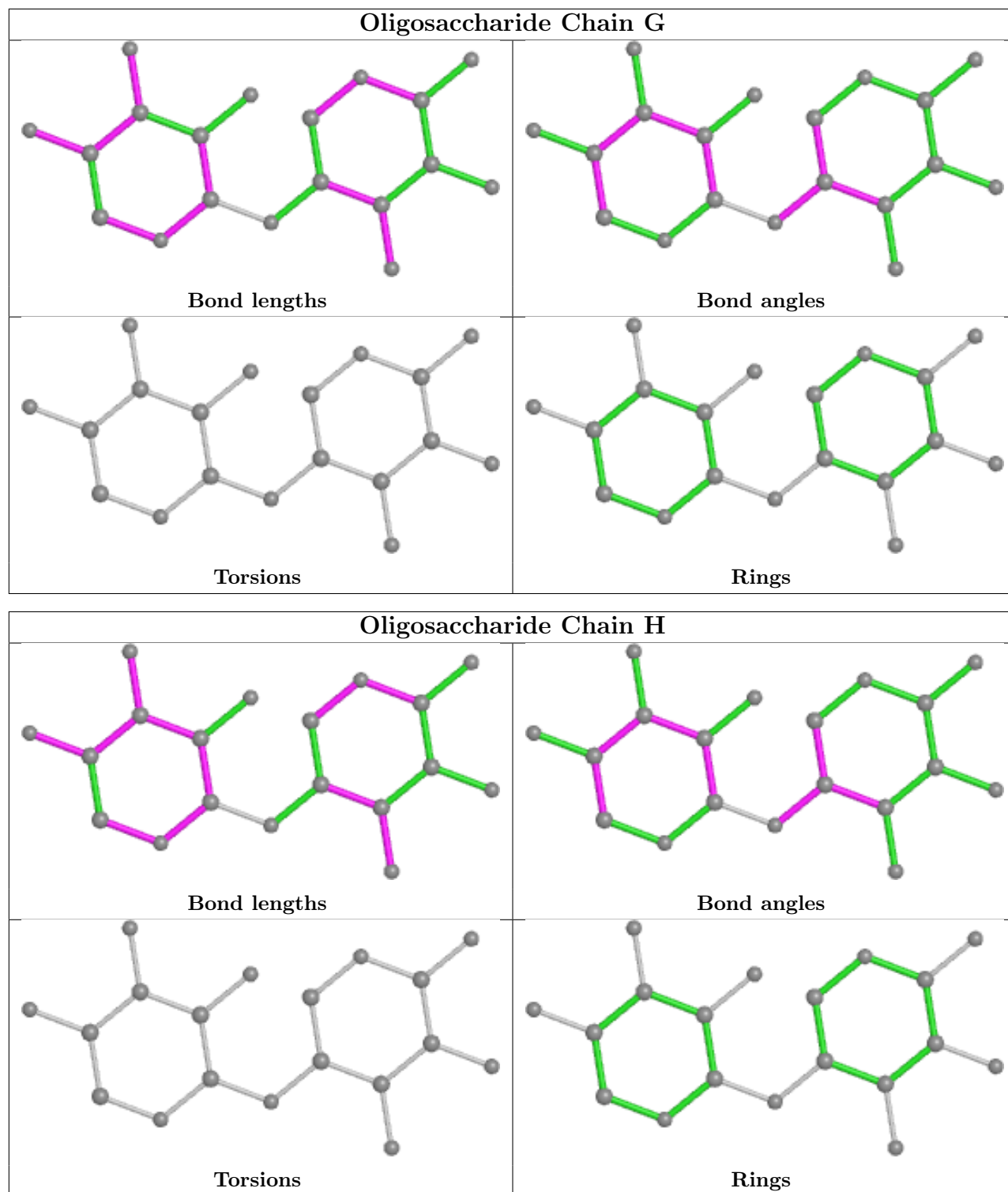
5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

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	536/541 (99%)	-0.28	4 (0%) 87	87	9, 22, 42, 54	0
1	B	533/541 (98%)	-0.10	11 (2%) 63	62	13, 26, 49, 73	0
1	C	535/541 (98%)	-0.26	4 (0%) 87	87	12, 24, 42, 57	0
1	D	533/541 (98%)	-0.32	5 (0%) 84	83	14, 24, 41, 59	0
All	All	2137/2164 (98%)	-0.24	24 (1%) 80	79	9, 24, 44, 73	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	447	ILE	4.6
1	A	272	SER	4.6
1	B	479	GLN	4.0
1	C	534	THR	4.0
1	B	1	MET	3.1
1	B	480	GLU	2.9
1	B	447	ILE	2.9
1	A	172	GLU	2.6
1	C	196	VAL	2.5
1	A	317	ALA	2.4
1	B	485	ASP	2.4
1	D	272	SER	2.3
1	C	447	ILE	2.3
1	B	360	PRO	2.2
1	D	271	SER	2.2
1	C	150	LYS	2.2
1	B	453	PRO	2.2
1	B	478	GLN	2.2
1	D	409	VAL	2.1
1	B	428	LEU	2.1
1	B	427	ALA	2.1

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Res	Type	RSRZ
1	B	334	LYS	2.1
1	A	320	VAL	2.1
1	D	426	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	XYP	G	2	9/10	0.96	0.16	15,16,18,21	0
2	XYP	G	1	10/10	0.97	0.11	17,18,22,27	0
2	XYP	F	1	10/10	0.97	0.09	15,17,20,21	0
2	XYP	E	1	10/10	0.98	0.11	15,16,20,20	0
2	XYP	F	2	9/10	0.98	0.12	13,16,18,18	0
2	XYP	H	1	10/10	0.98	0.07	14,15,18,19	0
2	XYP	H	2	9/10	0.98	0.12	13,15,17,18	0
2	XYP	E	2	9/10	0.99	0.15	14,15,17,17	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 E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
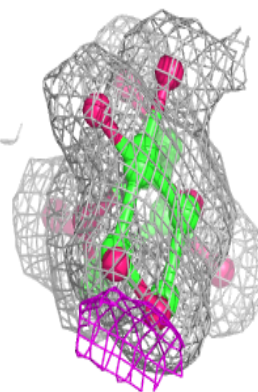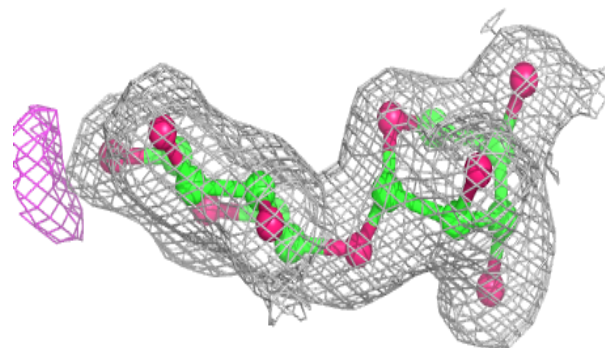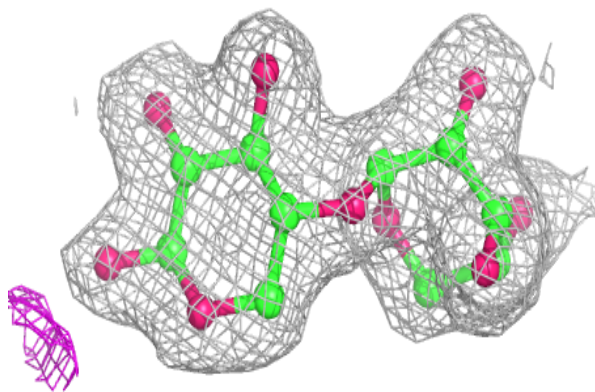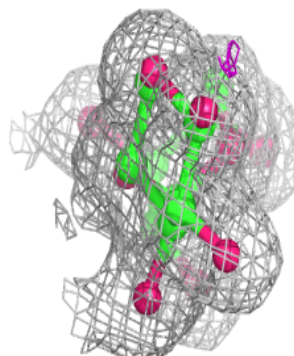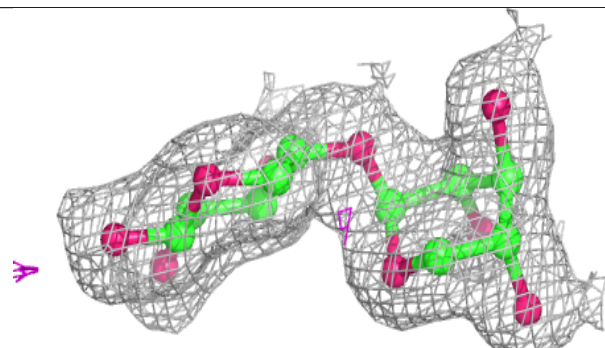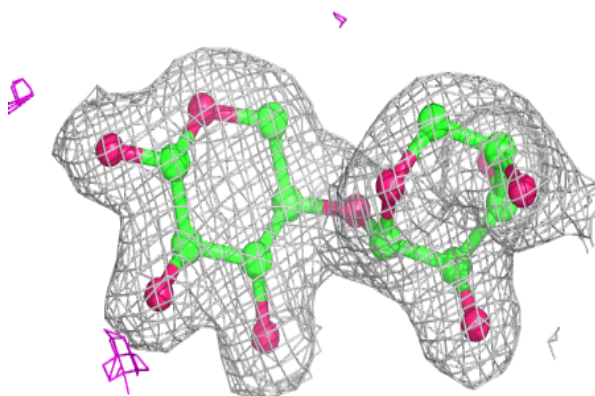and green (positive)
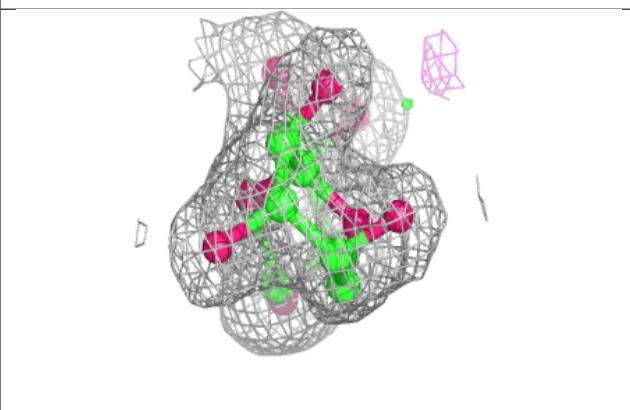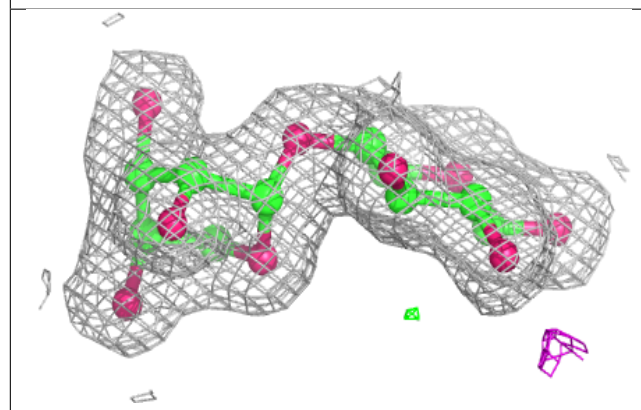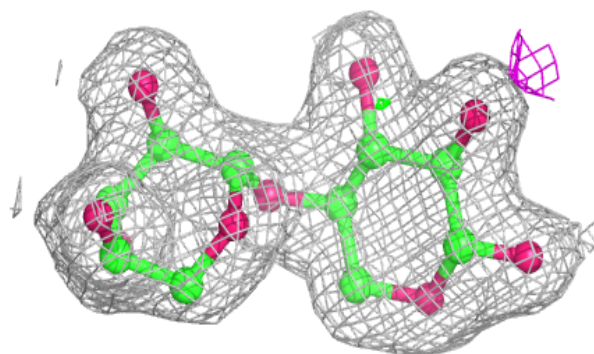
Electron density around Chain F:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
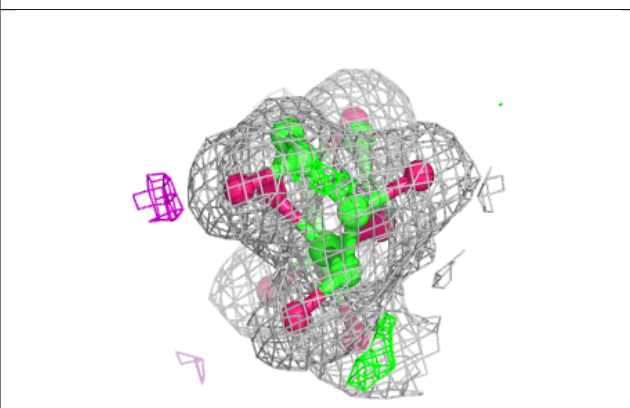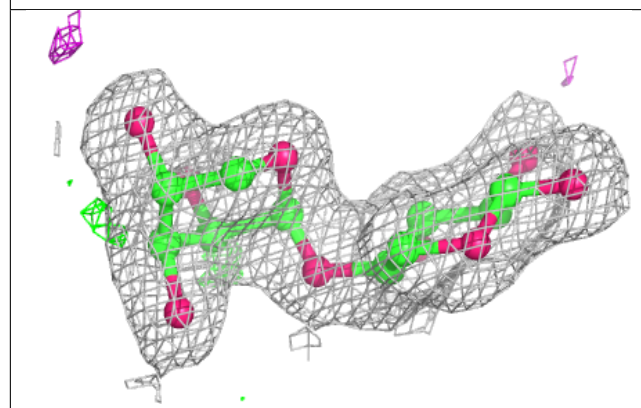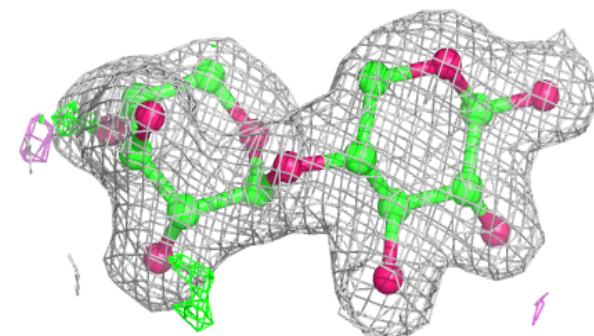
Electron density around Chain G:

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

Electron density around Chain H:

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

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.