



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:37 AM UTC

PDB ID : 5OLR / pdb_00005olr
Title : Rhamnogalacturonan lyase
Authors : Basle, A.; Luis, A.S.; Gilbert, H.J.
Deposited on : 2017-07-28
Resolution : 1.07 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:

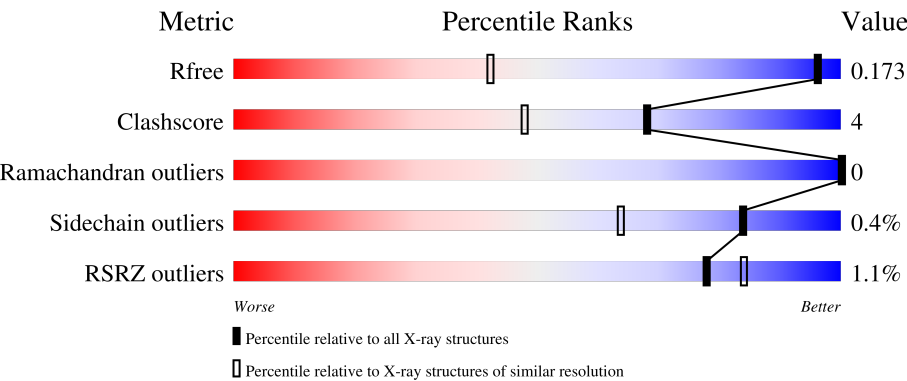
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.07 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	1687 (1.10-1.06)
Clashscore	190562	1727 (1.10-1.06)
Ramachandran outliers	187476	1679 (1.10-1.06)
Sidechain outliers	187428	1676 (1.10-1.06)
RSRZ outliers	180081	1687 (1.10-1.06)

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	78%19%
1	B	522	2% 80%19%
1	C	522	% 79%18%
2	D	3	67%33%
2	E	3	33%67%

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Mol	Chain	Length	Quality of chain
2	F	3	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11920 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 Rhamnogalacturonan lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	14	0
			3336	2105	566	645	20			
1	B	425	Total	C	N	O	S	0	13	0
			3333	2102	567	645	19			
1	C	426	Total	C	N	O	S	0	18	0
			3368	2123	572	654	19			

There are 30 discrepancies between the modelled and reference sequences:

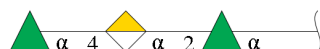
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	initiating methionine	UNP A0A139KMS2
A	23	GLY	-	expression tag	UNP A0A139KMS2
A	536	LEU	-	expression tag	UNP A0A139KMS2
A	537	GLU	-	expression tag	UNP A0A139KMS2
A	538	HIS	-	expression tag	UNP A0A139KMS2
A	539	HIS	-	expression tag	UNP A0A139KMS2
A	540	HIS	-	expression tag	UNP A0A139KMS2
A	541	HIS	-	expression tag	UNP A0A139KMS2
A	542	HIS	-	expression tag	UNP A0A139KMS2
A	543	HIS	-	expression tag	UNP A0A139KMS2
B	22	MET	-	initiating methionine	UNP A0A139KMS2
B	23	GLY	-	expression tag	UNP A0A139KMS2
B	536	LEU	-	expression tag	UNP A0A139KMS2
B	537	GLU	-	expression tag	UNP A0A139KMS2
B	538	HIS	-	expression tag	UNP A0A139KMS2
B	539	HIS	-	expression tag	UNP A0A139KMS2
B	540	HIS	-	expression tag	UNP A0A139KMS2
B	541	HIS	-	expression tag	UNP A0A139KMS2
B	542	HIS	-	expression tag	UNP A0A139KMS2
B	543	HIS	-	expression tag	UNP A0A139KMS2
C	22	MET	-	initiating methionine	UNP A0A139KMS2
C	23	GLY	-	expression tag	UNP A0A139KMS2
C	536	LEU	-	expression tag	UNP A0A139KMS2

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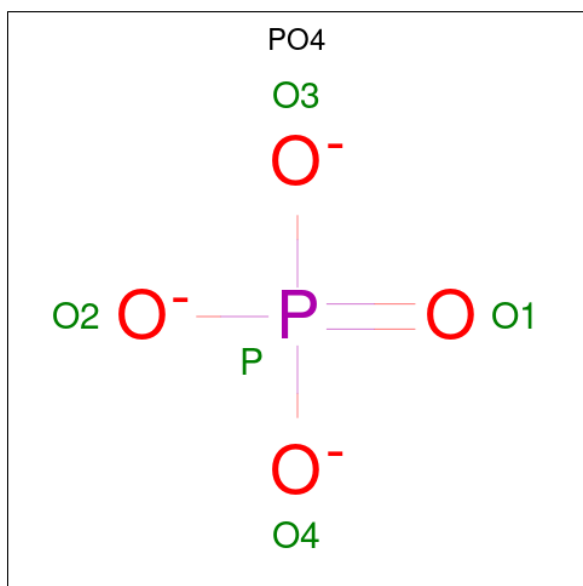
Chain	Residue	Modelled	Actual	Comment	Reference
C	537	GLU	-	expression tag	UNP A0A139KMS2
C	538	HIS	-	expression tag	UNP A0A139KMS2
C	539	HIS	-	expression tag	UNP A0A139KMS2
C	540	HIS	-	expression tag	UNP A0A139KMS2
C	541	HIS	-	expression tag	UNP A0A139KMS2
C	542	HIS	-	expression tag	UNP A0A139KMS2
C	543	HIS	-	expression tag	UNP A0A139KMS2

- Molecule 2 is an oligosaccharide called alpha-L-rhamnopyranose-(1-4)-alpha-D-galactopyranuronic acid-(1-2)-alpha-L-rhamnopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	3	Total	C	O	0	0	0
			33	18	15			
2	E	3	Total	C	O	0	0	0
			33	18	15			
2	F	3	Total	C	O	0	0	0
			33	18	15			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

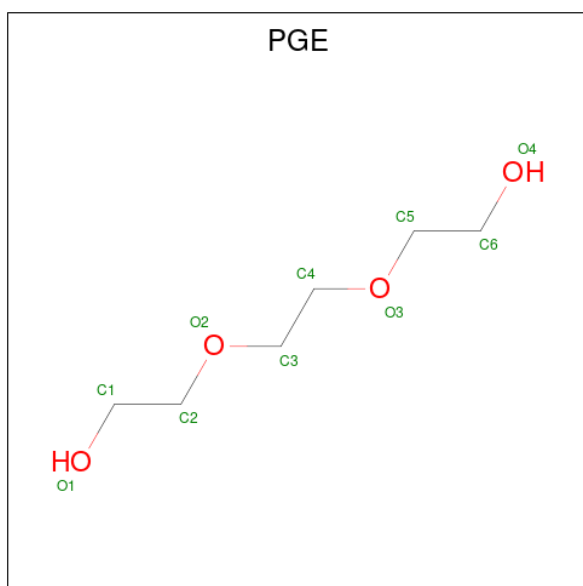


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ca 2 2	0	0
4	B	2	Total Ca 2 2	0	0
4	C	2	Total Ca 2 2	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).

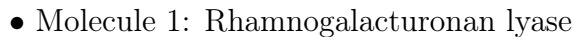


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 4 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	614	Total 614	O 614	0	0
6	B	539	Total 539	O 539	0	0
6	C	604	Total 604	O 604	0	0

- Molecule 1: Rhamnogalacturonan lyase



- Molecule 2: alpha-L-rhamnopyranose-(1-4)-alpha-D-galactopyranuronic acid-(1-2)-alpha-L-rhamnopyranose

Chain D:  67% 33%



- Molecule 2: alpha-L-rhamnopyranose-(1-4)-alpha-D-galactopyranuronic acid-(1-2)-alpha-L-rhamnopyranose

Chain E:  33% 67%



- Molecule 2: alpha-L-rhamnopyranose-(1-4)-alpha-D-galactopyranuronic acid-(1-2)-alpha-L-rhamnopyranose

Chain F:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.46Å 123.87Å 137.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.40 – 1.07 48.40 – 1.07	Depositor EDS
% Data completeness (in resolution range)	94.3 (48.40-1.07) 94.3 (48.40-1.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.07Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.145 , 0.166 0.154 , 0.173	Depositor DCC
R_{free} test set	26890 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	8.9	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11920	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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 57.82 % 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 2.2380e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADA, CA, PO4, RAM, PGE

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	0.67	0/3454	0.79	0/4674
1	B	0.71	1/3448 (0.0%)	0.81	0/4669
1	C	0.69	0/3498	0.79	0/4736
All	All	0.69	1/10400 (0.0%)	0.80	0/14079

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	423	ASN	CG-OD1	-5.51	1.13	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3336	0	3240	37	0
1	B	3333	0	3231	13	0
1	C	3368	0	3269	20	0
2	D	33	0	27	0	0
2	E	33	0	27	0	0
2	F	33	0	27	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	6	0	6	2	0
6	A	614	0	0	2	0
6	B	539	0	0	0	0
6	C	604	0	0	2	0
All	All	11920	0	9827	71	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 4.

All (71) 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:332[A]:PHE:CE2	1:A:346[A]:MET:HE1	1.62	1.34
1:A:330[B]:ILE:HD11	1:A:332[B]:PHE:CE2	1.69	1.27
1:A:332[B]:PHE:CE2	1:A:346[B]:MET:HE1	1.77	1.20
1:A:330[B]:ILE:CD1	1:A:332[B]:PHE:CE2	2.25	1.18
1:A:330[B]:ILE:HD11	1:A:332[B]:PHE:CZ	1.81	1.15
1:A:330[B]:ILE:CD1	1:A:332[B]:PHE:CZ	2.30	1.14
1:A:332[A]:PHE:CD2	1:A:346[A]:MET:HE1	1.83	1.13
1:B:330[B]:ILE:HD11	1:B:332[B]:PHE:CE2	1.88	1.09
1:C:330[B]:ILE:HD11	1:C:332[B]:PHE:CE2	1.88	1.09
1:C:330[B]:ILE:CD1	1:C:332[B]:PHE:CE2	2.38	1.06
1:C:330[B]:ILE:CD1	1:C:332[B]:PHE:CZ	2.38	1.04
1:B:330[B]:ILE:CD1	1:B:332[B]:PHE:CE2	2.43	1.01
1:C:330[B]:ILE:HD11	1:C:332[B]:PHE:CZ	1.94	1.01
1:A:332[B]:PHE:CD2	1:A:346[B]:MET:HE1	1.98	0.98
1:B:330[B]:ILE:HD11	1:B:332[B]:PHE:CZ	1.99	0.97
1:B:330[B]:ILE:CD1	1:B:332[B]:PHE:CZ	2.50	0.94
1:A:330[B]:ILE:HD12	1:A:332[B]:PHE:CZ	2.05	0.91
1:A:332[A]:PHE:HE2	1:A:346[A]:MET:HE1	1.16	0.90
1:A:330[B]:ILE:HD11	1:A:332[B]:PHE:HE2	1.30	0.89
1:A:366[B]:MET:SD	1:A:368:LYS:HD3	2.12	0.89
1:A:330[B]:ILE:CG1	1:A:332[B]:PHE:CE2	2.55	0.88
1:C:330[B]:ILE:HD12	1:C:332[B]:PHE:CZ	2.07	0.88
1:A:330[B]:ILE:HG13	1:A:332[B]:PHE:CE2	2.10	0.87
1:A:332[A]:PHE:CE2	1:A:346[A]:MET:CE	2.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330[B]:ILE:HG13	1:C:332[B]:PHE:CE2	2.12	0.85
1:B:330[B]:ILE:HD11	1:B:332[B]:PHE:HE2	1.46	0.81
1:C:330[B]:ILE:CG1	1:C:332[B]:PHE:CE2	2.63	0.80
1:A:366[B]:MET:SD	1:A:368:LYS:CD	2.70	0.80
1:A:332[A]:PHE:HE2	1:A:346[A]:MET:CE	1.94	0.78
1:B:330[B]:ILE:HG13	1:B:332[B]:PHE:CE2	2.19	0.77
1:B:330[B]:ILE:CG1	1:B:332[B]:PHE:CE2	2.68	0.76
1:A:332[B]:PHE:HE2	1:A:346[B]:MET:HE1	1.47	0.72
1:B:330[B]:ILE:HD12	1:B:332[B]:PHE:CZ	2.25	0.71
1:C:330[B]:ILE:HD11	1:C:332[B]:PHE:HE2	1.49	0.71
1:A:332[A]:PHE:CD2	1:A:346[A]:MET:CE	2.70	0.68
1:A:301[A]:SER:OG	6:A:701:HOH:O	1.95	0.67
1:C:330[B]:ILE:HD11	1:C:332[B]:PHE:HZ	1.59	0.67
1:A:330[B]:ILE:HD11	1:A:332[B]:PHE:HZ	1.54	0.66
1:A:330[B]:ILE:CD1	1:A:332[B]:PHE:HZ	2.01	0.65
1:A:330[B]:ILE:CG1	1:A:332[B]:PHE:HE2	2.09	0.64
1:C:330[B]:ILE:CD1	1:C:332[B]:PHE:HZ	2.07	0.61
1:A:332[B]:PHE:CE2	1:A:346[B]:MET:CE	2.70	0.61
1:A:330[B]:ILE:CD1	1:A:332[B]:PHE:HE2	1.93	0.58
1:A:319:ARG:HH12	5:A:607:PGE:H3	1.71	0.56
1:C:401[B]:GLU:OE2	1:C:441:ARG:NH1	2.36	0.55
1:A:207:GLU:O	1:A:210[B]:LYS:HG2	2.07	0.54
1:A:366[A]:MET:HE1	1:A:391[A]:GLU:OE2	2.07	0.53
1:C:330[B]:ILE:CD1	1:C:332[B]:PHE:HE2	2.08	0.52
1:C:330[B]:ILE:CG1	1:C:332[B]:PHE:HE2	2.18	0.52
1:B:330[B]:ILE:CG1	1:B:332[B]:PHE:HE2	2.22	0.51
1:A:332[B]:PHE:CD2	1:A:346[B]:MET:CE	2.86	0.50
1:B:330[B]:ILE:CD1	1:B:332[B]:PHE:HZ	2.22	0.49
1:B:330[B]:ILE:HD11	1:B:332[B]:PHE:HZ	1.68	0.49
1:A:332[A]:PHE:HD2	1:A:346[A]:MET:HE1	1.60	0.49
1:C:121:PRO:HD2	1:C:126[B]:ILE:HD11	1.95	0.48
1:A:310[A]:ASN:HA	1:A:334:SER:O	2.14	0.47
1:A:332[A]:PHE:HD2	1:A:346[A]:MET:CE	2.23	0.47
1:C:296:LEU:HD22	1:C:353:LEU:HG	1.96	0.47
5:A:607:PGE:C6	6:A:713:HOH:O	2.62	0.47
1:C:375:THR:HG21	1:C:405[B]:GLU:CG	2.44	0.47
1:C:199:TYR:HA	1:C:242:TRP:O	2.15	0.47
1:A:330[B]:ILE:HG13	1:A:332[B]:PHE:CD2	2.49	0.46
1:C:242:TRP:HA	1:C:266:PHE:O	2.17	0.44
1:A:366[B]:MET:SD	1:A:368:LYS:HG3	2.58	0.43
1:C:412[A]:GLU:HG3	6:C:1200:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:TYR:HA	1:B:242:TRP:O	2.18	0.42
1:B:366[B]:MET:HE1	1:B:391[B]:GLU:OE1	2.19	0.42
1:A:199:TYR:HA	1:A:242:TRP:O	2.20	0.42
1:A:431:PHE:CD1	1:A:431:PHE:C	2.98	0.41
1:A:139:LYS:HA	1:A:171:GLU:O	2.21	0.40
1:C:275:LYS:HE3	6:C:704:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/522 (84%)	430 (98%)	7 (2%)	0	100	100
1	B	436/522 (84%)	429 (98%)	7 (2%)	0	100	100
1	C	442/522 (85%)	435 (98%)	7 (2%)	0	100	100
All	All	1315/1566 (84%)	1294 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	368/436 (84%)	367 (100%)	1 (0%)	86	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	367/436 (84%)	364 (99%)	3 (1%)	73	42
1	C	372/436 (85%)	372 (100%)	0	100	100
All	All	1107/1308 (85%)	1103 (100%)	4 (0%)	84	64

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	315	TYR
1	B	315	TYR
1	B	333	GLU
1	B	412	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	200	ASN
1	B	107	ASN
1	B	310	ASN
1	C	51	GLN
1	C	109	GLN
1	C	324	ASN
1	C	394	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 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	RAM	D	1	2	11,11,11	0.51	0	16,16,16	0.76	1 (6%)
2	ADA	D	2	2	12,12,13	0.78	0	14,17,19	0.51	0
2	RAM	D	3	2	10,10,11	0.74	0	14,14,16	0.81	0
2	RAM	E	1	2	11,11,11	0.51	0	16,16,16	0.69	0
2	ADA	E	2	2	12,12,13	0.93	1 (8%)	14,17,19	0.71	0
2	RAM	E	3	2	10,10,11	0.83	0	14,14,16	0.89	1 (7%)
2	RAM	F	1	2	11,11,11	0.55	0	16,16,16	0.64	0
2	ADA	F	2	2	12,12,13	0.88	0	14,17,19	0.59	0
2	RAM	F	3	2	10,10,11	0.75	0	14,14,16	0.70	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	RAM	D	1	2	-	-	0/1/1/1
2	ADA	D	2	2	-	0/4/21/24	0/1/1/1
2	RAM	D	3	2	-	-	0/1/1/1
2	RAM	E	1	2	-	-	0/1/1/1
2	ADA	E	2	2	-	0/4/21/24	0/1/1/1
2	RAM	E	3	2	-	-	0/1/1/1
2	RAM	F	1	2	-	-	0/1/1/1
2	ADA	F	2	2	-	0/4/21/24	0/1/1/1
2	RAM	F	3	2	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	ADA	O6B-C6	-2.20	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	RAM	O5-C1-C2	2.20	116.04	110.79
2	D	1	RAM	O2-C2-C1	-2.09	104.43	109.25

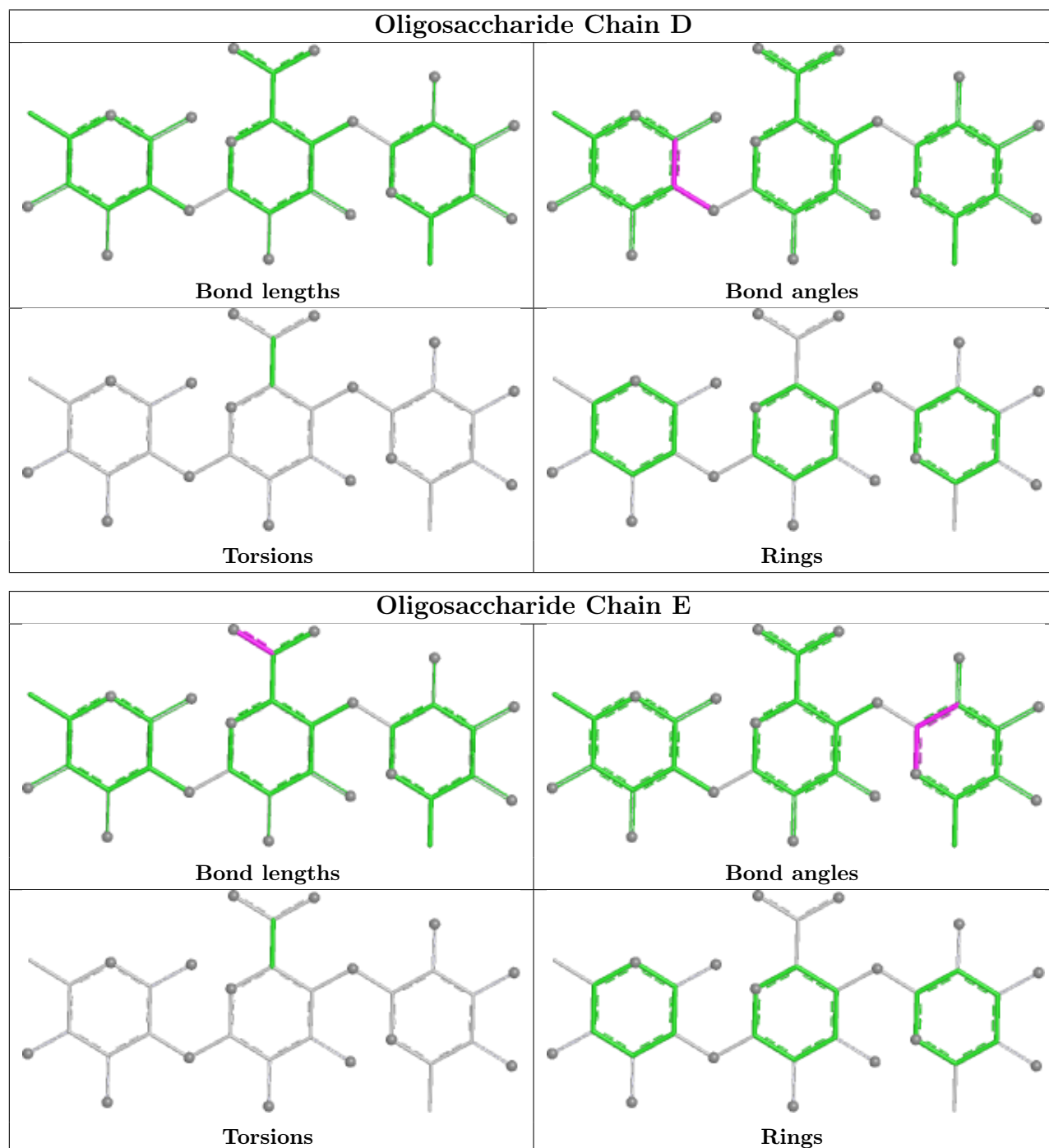
There are no chirality outliers.

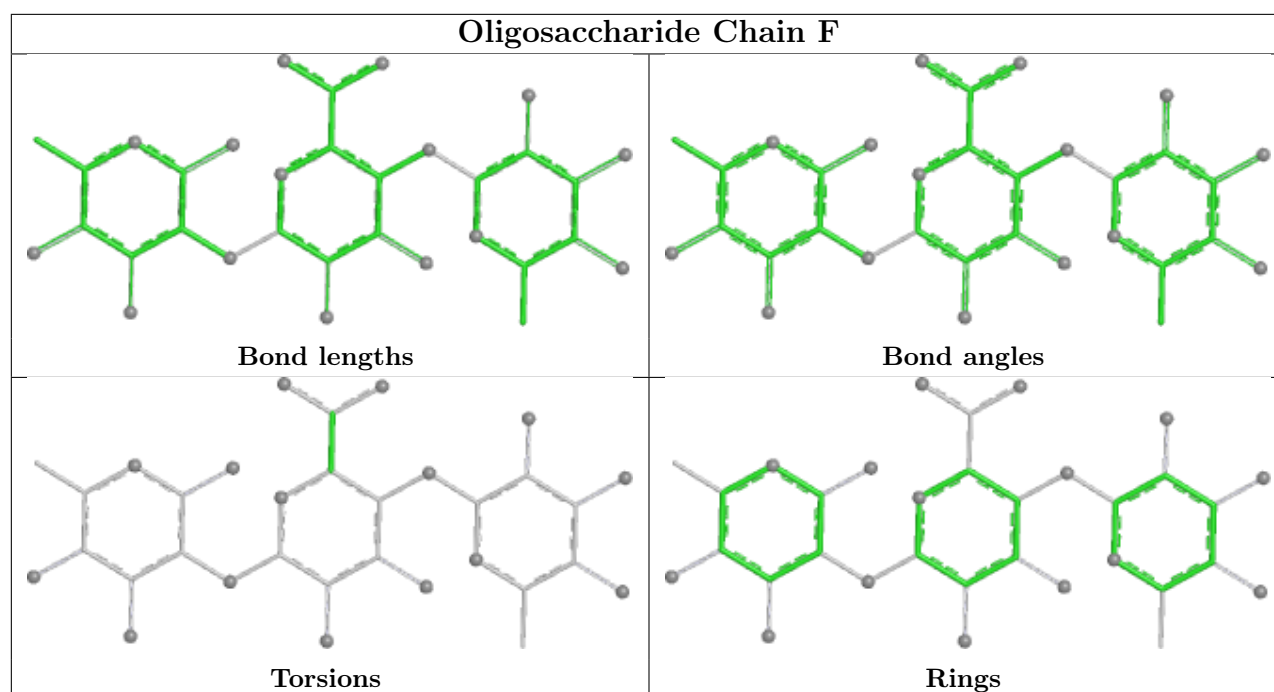
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	A	601	4	4,4,4	1.40	0	6,6,6	1.18	1 (16%)
3	PO4	C	601	4	4,4,4	1.29	0	6,6,6	1.09	0
5	PGE	A	607	-	5,5,9	0.94	0	4,4,8	3.44	2 (50%)
3	PO4	B	601	4	4,4,4	1.03	0	6,6,6	0.91	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	A	607	-	-	1/3/3/7	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	607	PGE	C5-O3-C4	-6.34	90.81	113.06
5	A	607	PGE	O3-C4-C3	2.57	121.44	110.11
3	A	601	PO4	O4-P-O2	2.19	114.73	107.91

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	607	PGE	O2-C3-C4-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	607	PGE	2	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	425/522 (81%)	-0.22	1 (0%) 91 92	4, 9, 18, 27	14 (3%)
1	B	425/522 (81%)	-0.04	9 (2%) 63 70	4, 10, 22, 37	13 (3%)
1	C	426/522 (81%)	-0.25	4 (0%) 81 86	4, 9, 17, 30	18 (4%)
All	All	1276/1566 (81%)	-0.17	14 (1%) 78 84	4, 9, 20, 37	45 (3%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	422	PRO	3.3
1	C	449	ALA	3.0
1	C	436	THR	2.9
1	B	440	LEU	2.9
1	C	437	ASP	2.9
1	B	443	TRP	2.8
1	A	41	ASP	2.6
1	B	208	GLY	2.5
1	B	421	LYS	2.5
1	B	436	THR	2.4
1	B	35	SER	2.1
1	B	109	GLN	2.1
1	C	41	ASP	2.1
1	B	41	ASP	2.0

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

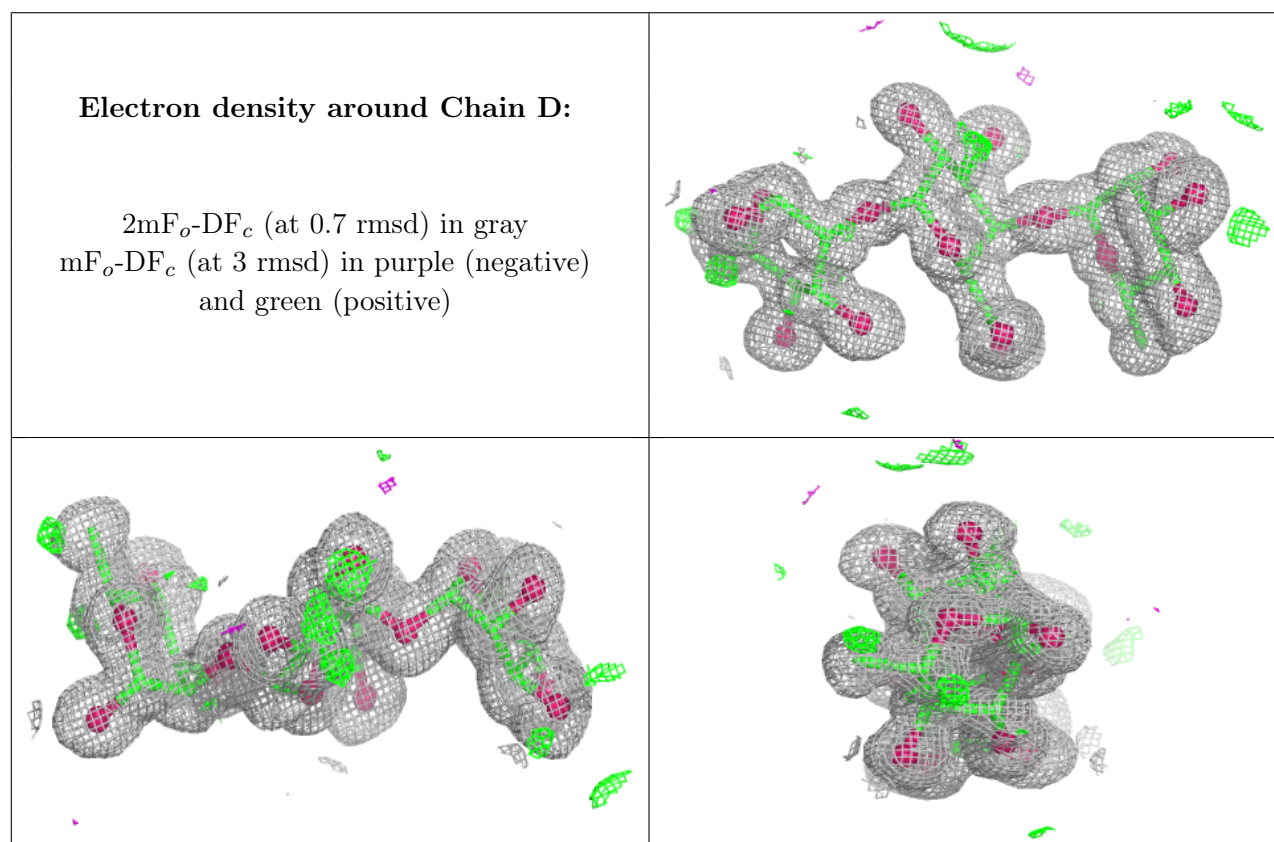
There are no non-standard protein/DNA/RNA residues in this entry.

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.

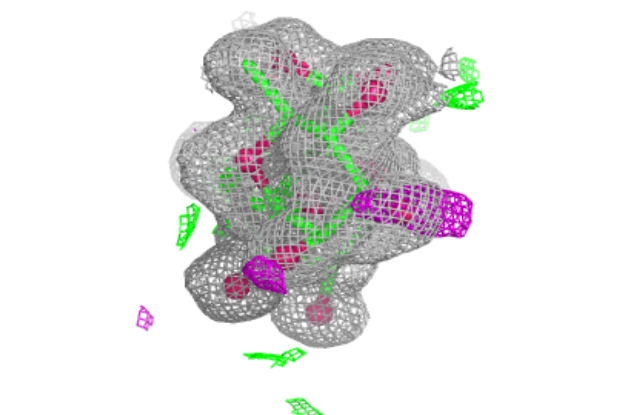
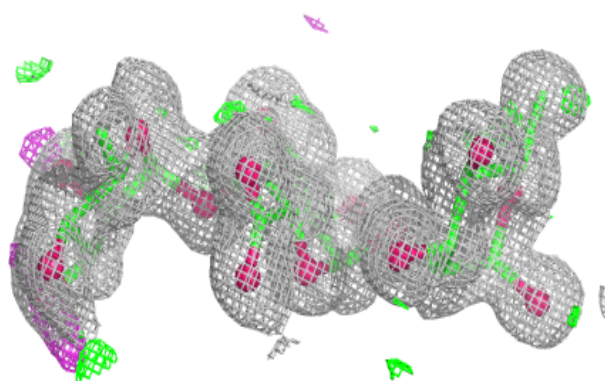
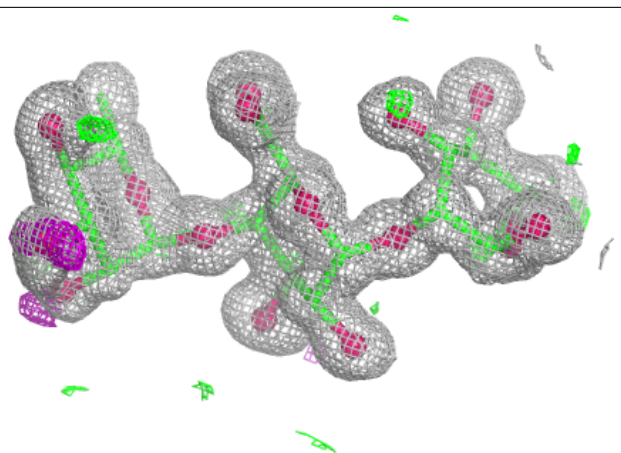
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	RAM	E	3	10/11	0.92	0.09	17,20,27,28	0
2	RAM	D	3	10/11	0.96	0.08	11,14,18,21	0
2	RAM	F	3	10/11	0.97	0.06	12,15,20,21	0
2	RAM	E	1	11/11	0.98	0.05	8,9,10,10	0
2	ADA	E	2	12/13	0.98	0.05	10,11,14,14	0
2	ADA	D	2	12/13	0.99	0.04	8,9,10,10	0
2	RAM	F	1	11/11	0.99	0.03	6,7,8,8	0
2	ADA	F	2	12/13	0.99	0.03	8,9,10,11	0
2	RAM	D	1	11/11	0.99	0.03	6,7,8,8	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.

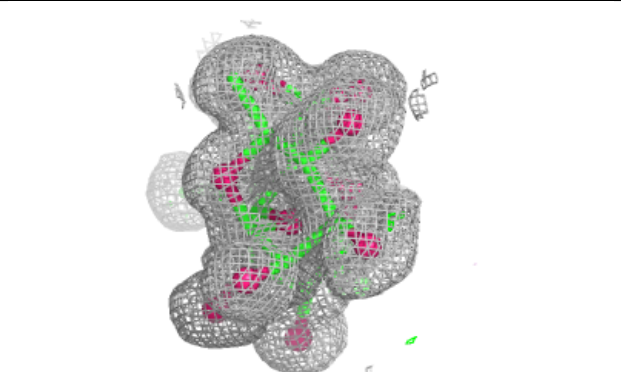
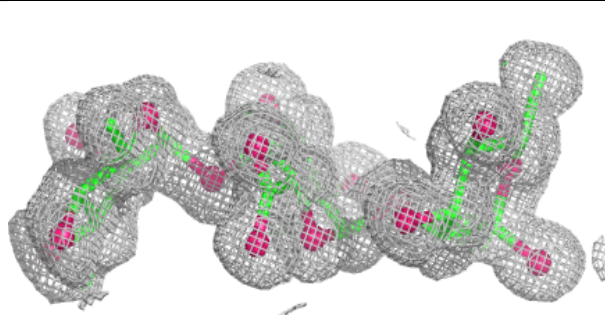
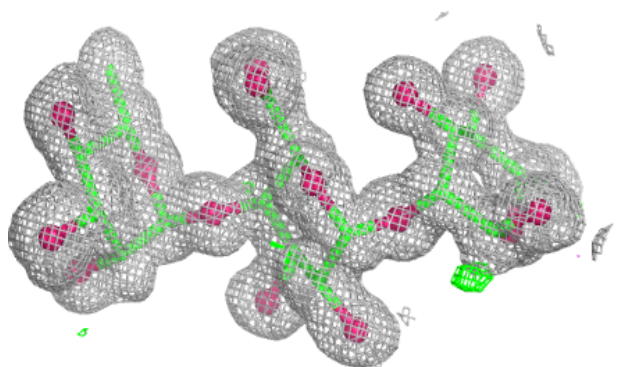


Electron density around Chain E:

$2mF_o-DF_c$ (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)



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PGE	A	607	6/10	0.89	0.13	11,13,18,31	0
3	PO4	B	601	5/5	0.99	0.04	7,8,9,10	0
3	PO4	C	601	5/5	1.00	0.03	6,7,9,10	0
4	CA	A	602	1/1	1.00	0.05	10,10,10,10	0
4	CA	A	603	1/1	1.00	0.01	5,5,5,5	0
4	CA	B	602	1/1	1.00	0.06	11,11,11,11	0
4	CA	B	603	1/1	1.00	0.00	6,6,6,6	0
4	CA	C	602	1/1	1.00	0.01	5,5,5,5	0
4	CA	C	603	1/1	1.00	0.03	9,9,9,9	0
3	PO4	A	601	5/5	1.00	0.03	6,7,9,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.