



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 07:38 PM BST

PDB ID : 6RQX
Title : High-resolution crystal structure of ERAP1 in complex with 10mer phosphinic peptide
Authors : Giastas, P.; Stratikos, E.
Deposited on : 2019-05-16
Resolution : 1.68 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

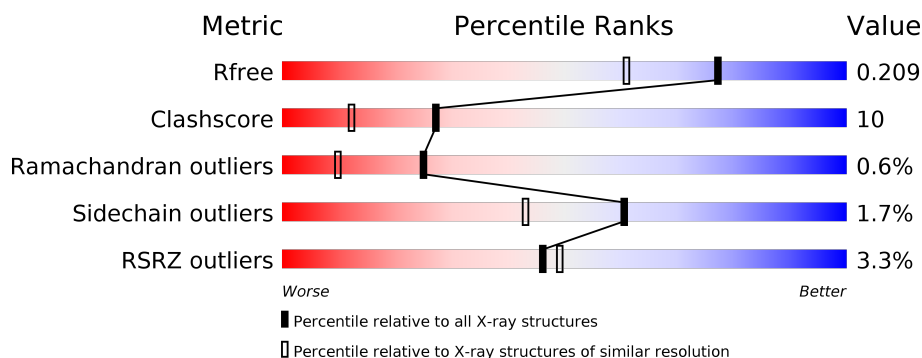
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>8%</div> </div> </div>
2	B	9	<div> <div>44%</div> <div> <div></div> <div>56%</div> <div>44%</div> </div> </div>
3	C	3	<div> <div>67%</div> <div>33%</div> </div>
4	D	4	<div> <div>50%</div> <div>50%</div> </div>
5	E	2	<div> <div>50%</div> <div>50%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PGE	A	1050	-	-	X	-
4	BMA	D	3	-	-	-	X
4	MAN	D	4	-	-	-	X
5	NAG	E	2	-	-	-	X
8	SCN	A	1015	-	-	X	-
8	SCN	A	1016	-	-	X	-
9	EDO	A	1042	-	-	-	X
9	EDO	A	1043	-	-	X	-
9	EDO	A	1044	-	-	-	X

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 8315 atoms, of which 174 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.

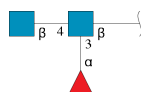
- Molecule 1 is a protein called Endoplasmic reticulum aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	862	Total	C	N	O	S	5	21	0
			7026	4529	1155	1307	35			

- Molecule 2 is a protein called PSE-LYS-HIS-HIS-ALA-PHE-SER-PHE-LYS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	P	0	0	0
			93	64	15	13	1			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



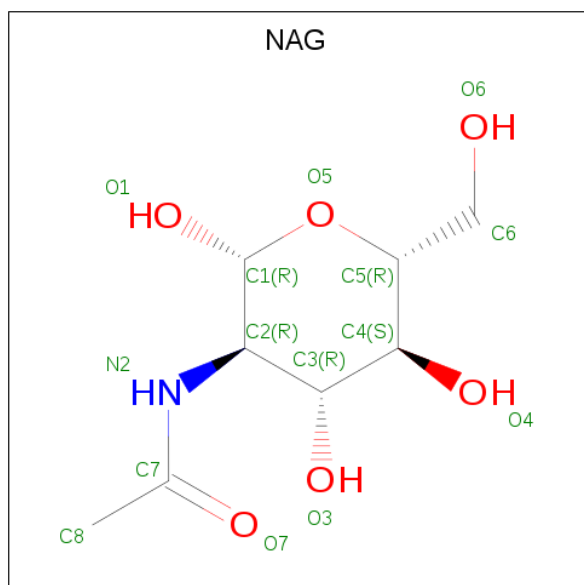
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		

- Molecule 8 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	S	0	0
			3	1	1	1		
8	A	1	Total	C	N	S	0	0
			3	1	1	1		
8	A	1	Total	C	N	S	0	0
			3	1	1	1		
8	A	1	Total	C	N	S	0	0
			3	1	1	1		
8	A	1	Total	C	N	S	0	0
			3	1	1	1		
8	A	1	Total	C	N	S	0	0
			3	1	1	1		
8	A	1	Total	C	N	S	0	0
			3	1	1	1		
8	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	A	1	Total	C	H	O	0	0
			10	2	6	2		

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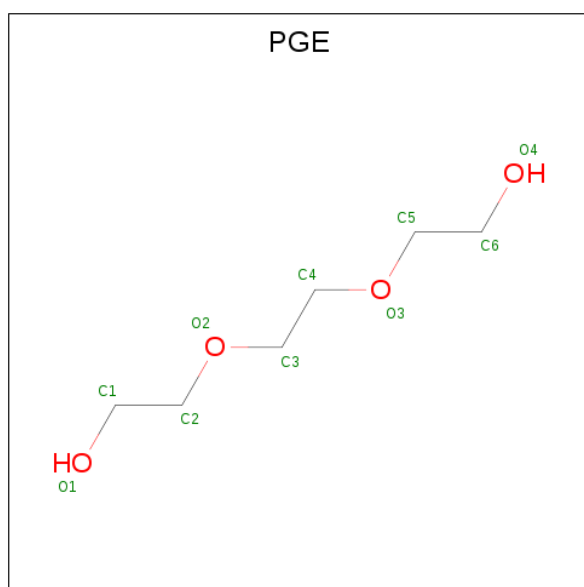
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	4	Total	Na	0	0
			4	4		

- Molecule 11 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			24	6	14	4		
11	A	1	Total	C	H	O	0	0
			24	6	14	4		
11	A	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	725	Total	O	0	0
			725	725		
12	B	11	Total	O	0	0
			11	11		

- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	58.00Å 116.44Å 147.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.68 – 1.68 73.68 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.7 (73.68-1.68) 99.7 (73.68-1.68)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.68Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.176 , 0.209 0.176 , 0.209	Depositor DCC
R_{free} test set	2000 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8315	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SCN, KF2, NAG, NA, EDO, PGE, BMA, MAN, FUC

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	0.38	0/7261	0.54	0/9841
2	B	0.45	0/75	0.57	0/96
All	All	0.39	0/7336	0.54	0/9937

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	7026	0	6988	145	0
2	B	93	0	68	11	0
3	C	38	0	34	0	0
4	D	50	0	43	1	0
5	E	28	0	25	1	0
6	A	14	0	13	0	0
7	A	1	0	0	0	0
8	A	33	0	0	5	0
9	A	88	132	131	16	0
10	A	4	0	0	0	0
11	A	30	42	42	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	A	725	0	0	27	3
12	B	11	0	0	0	0
All	All	8141	174	7344	149	3

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 10.

The worst 5 of 149 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:550:MET:SD	12:A:1601:HOH:O	2.11	1.07
1:A:170:LYS:NZ	12:A:1103:HOH:O	1.92	1.03
1:A:809:GLN:NE2	12:A:1105:HOH:O	1.99	0.95
1:A:856:ASN:OD1	12:A:1102:HOH:O	1.90	0.89
1:A:909:GLN:OE1	12:A:1104:HOH:O	1.94	0.85

All (3) 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)
12:A:1413:HOH:O	12:A:1413:HOH:O[2_51111]	2.03	0.17
12:A:1432:HOH:O	12:A:1715:HOH:O[3_-16411]	2.05	0.15
12:A:1572:HOH:O	12:A:1651:HOH:O[3_-16511]	2.07	0.13

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	877/938 (94%)	844 (96%)	28 (3%)	5 (1%)	25	10
2	B	7/9 (78%)	5 (71%)	2 (29%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	884/947 (93%)	849 (96%)	30 (3%)	5 (1%)	25	10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	ALA
1	A	936	GLU
1	A	453	SER
1	A	559	THR
1	A	865	GLU

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	786/836 (94%)	771 (98%)	15 (2%)	57	38
2	B	7/7 (100%)	7 (100%)	0	100	100
All	All	793/843 (94%)	778 (98%)	15 (2%)	60	38

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	366[B]	MET
1	A	550	MET
1	A	723[A]	SER
1	A	366[A]	MET
1	A	713	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	856	ASN
1	A	909	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 ⓘ

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	$\# Z > 2$
3	NAG	C	1	1,3	14,14,15	0.44	0	17,19,21	0.71	1 (5%)
3	FUC	C	2	3	10,10,11	0.63	0	14,14,16	0.78	0
3	NAG	C	3	3	14,14,15	0.30	0	17,19,21	0.36	0
4	NAG	D	1	1,4	14,14,15	0.20	0	17,19,21	0.46	0
4	NAG	D	2	4	14,14,15	0.38	0	17,19,21	0.46	0
4	BMA	D	3	4	11,11,12	0.74	0	15,15,17	0.69	0
4	MAN	D	4	4	11,11,12	1.09	1 (9%)	15,15,17	0.83	0
5	NAG	E	1	1,5	14,14,15	0.33	0	17,19,21	0.48	0
5	NAG	E	2	5	14,14,15	0.33	0	17,19,21	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1
3	NAG	C	3	3	-	0/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4	MAN	O5-C1	-2.04	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	2.23	115.21	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

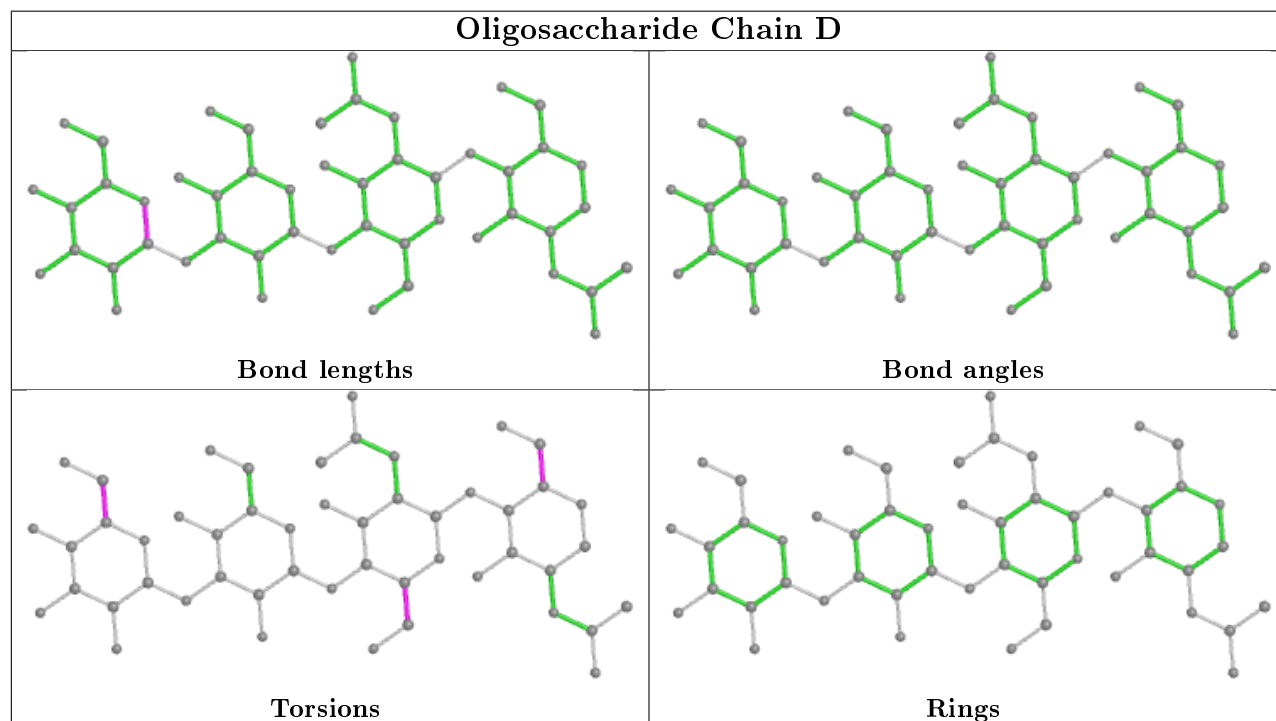
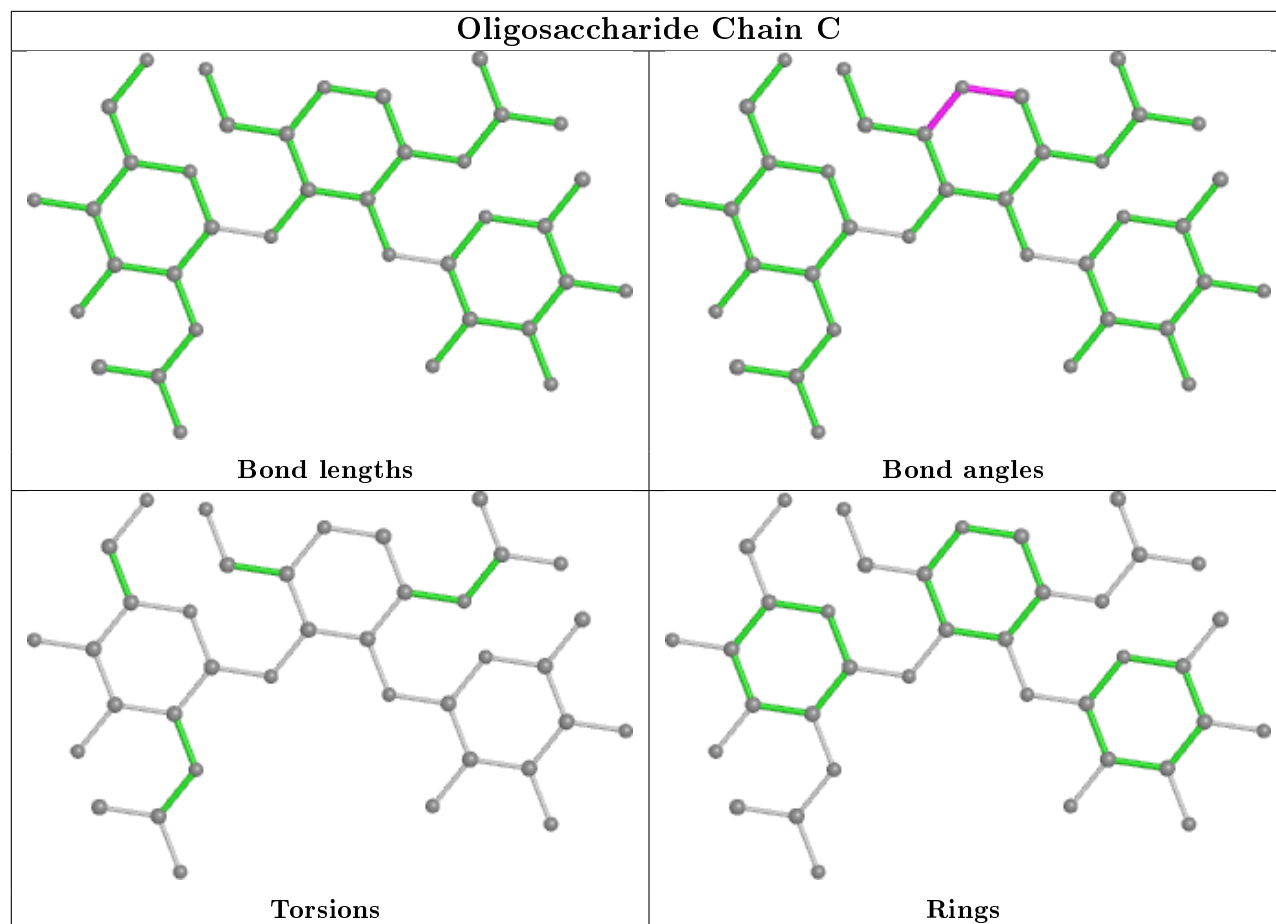
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6

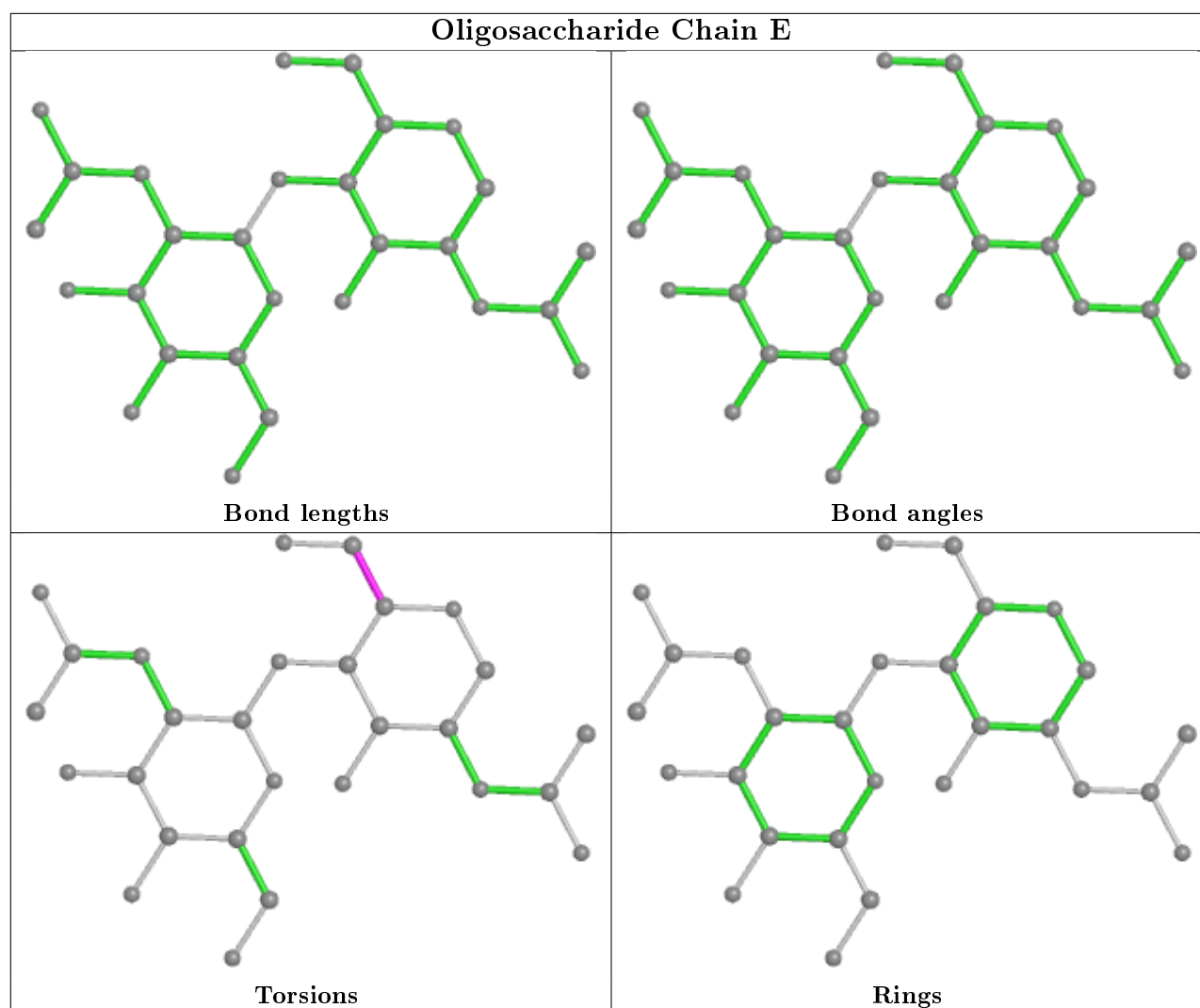
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	NAG	1	0
4	D	1	NAG	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 ⓘ

Of 42 ligands modelled in this entry, 5 are monoatomic - leaving 37 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	$\# Z > 2$
6	NAG	A	1010	1	14,14,15	0.16	0	17,19,21	0.57	0
9	EDO	A	1035	-	3,3,3	0.50	0	2,2,2	0.26	0
8	SCN	A	1022	-	1,2,2	0.93	0	0,1,1	0.00	-
9	EDO	A	1042	-	3,3,3	0.51	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	A	1040	-	3,3,3	0.51	0	2,2,2	0.25	0
9	EDO	A	1024	-	3,3,3	0.47	0	2,2,2	0.49	0
8	SCN	A	1012	-	1,2,2	1.10	0	0,1,1	0.00	-
9	EDO	A	1031	-	3,3,3	0.50	0	2,2,2	0.27	0
11	PGE	A	1050	-	9,9,9	0.39	0	8,8,8	0.39	0
8	SCN	A	1017	-	1,2,2	0.83	0	0,1,1	0.00	-
9	EDO	A	1044	-	3,3,3	0.96	0	2,2,2	0.07	0
8	SCN	A	1021	-	1,2,2	0.93	0	0,1,1	0.00	-
9	EDO	A	1034	-	3,3,3	0.45	0	2,2,2	0.45	0
9	EDO	A	1030	-	3,3,3	0.44	0	2,2,2	0.30	0
9	EDO	A	1028	-	3,3,3	0.53	0	2,2,2	0.16	0
8	SCN	A	1015	-	1,2,2	0.88	0	0,1,1	0.00	-
9	EDO	A	1023	-	3,3,3	0.43	0	2,2,2	0.45	0
9	EDO	A	1037	-	3,3,3	0.48	0	2,2,2	0.31	0
9	EDO	A	1036	-	3,3,3	0.49	0	2,2,2	0.29	0
8	SCN	A	1013	-	1,2,2	0.85	0	0,1,1	0.00	-
9	EDO	A	1032	-	3,3,3	0.47	0	2,2,2	0.45	0
9	EDO	A	1041	-	3,3,3	0.35	0	2,2,2	0.56	0
8	SCN	A	1014	-	1,2,2	1.18	0	0,1,1	0.00	-
9	EDO	A	1033	-	3,3,3	0.44	0	2,2,2	0.45	0
11	PGE	A	1049	-	9,9,9	0.30	0	8,8,8	0.43	0
9	EDO	A	1025	-	3,3,3	0.35	0	2,2,2	0.70	0
11	PGE	A	1051	-	9,9,9	0.31	0	8,8,8	0.37	0
8	SCN	A	1020	-	1,2,2	0.98	0	0,1,1	0.00	-
8	SCN	A	1018	-	1,2,2	0.91	0	0,1,1	0.00	-
8	SCN	A	1016	-	1,2,2	1.02	0	0,1,1	0.00	-
9	EDO	A	1027	-	3,3,3	0.44	0	2,2,2	0.61	0
8	SCN	A	1019	-	1,2,2	0.93	0	0,1,1	0.00	-
9	EDO	A	1026	-	3,3,3	0.50	0	2,2,2	0.54	0
9	EDO	A	1039	-	3,3,3	0.49	0	2,2,2	0.26	0
9	EDO	A	1038	-	3,3,3	0.55	0	2,2,2	0.09	0
9	EDO	A	1029	-	3,3,3	0.41	0	2,2,2	0.43	0
9	EDO	A	1043	-	3,3,3	0.47	0	2,2,2	0.26	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
6	NAG	A	1010	1	-	0/6/23/26	0/1/1/1
9	EDO	A	1035	-	-	1/1/1/1	-
9	EDO	A	1042	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	1040	-	-	0/1/1/1	-
9	EDO	A	1024	-	-	0/1/1/1	-
9	EDO	A	1031	-	-	0/1/1/1	-
11	PGE	A	1050	-	-	4/7/7/7	-
9	EDO	A	1044	-	-	0/1/1/1	-
9	EDO	A	1034	-	-	0/1/1/1	-
9	EDO	A	1030	-	-	0/1/1/1	-
9	EDO	A	1028	-	-	1/1/1/1	-
9	EDO	A	1039	-	-	0/1/1/1	-
9	EDO	A	1023	-	-	0/1/1/1	-
9	EDO	A	1036	-	-	1/1/1/1	-
9	EDO	A	1037	-	-	0/1/1/1	-
9	EDO	A	1032	-	-	1/1/1/1	-
9	EDO	A	1041	-	-	1/1/1/1	-
9	EDO	A	1033	-	-	0/1/1/1	-
11	PGE	A	1049	-	-	5/7/7/7	-
9	EDO	A	1025	-	-	0/1/1/1	-
11	PGE	A	1051	-	-	4/7/7/7	-
9	EDO	A	1027	-	-	0/1/1/1	-
9	EDO	A	1026	-	-	1/1/1/1	-
9	EDO	A	1038	-	-	1/1/1/1	-
9	EDO	A	1029	-	-	0/1/1/1	-
9	EDO	A	1043	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	1049	PGE	O2-C3-C4-O3
11	A	1050	PGE	O2-C3-C4-O3
11	A	1049	PGE	O3-C5-C6-O4
11	A	1050	PGE	O3-C5-C6-O4
11	A	1051	PGE	O3-C5-C6-O4

There are no ring outliers.

15 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1050	PGE	11	0
9	A	1034	EDO	1	0
9	A	1030	EDO	2	0
9	A	1028	EDO	2	0
8	A	1015	SCN	2	0
9	A	1023	EDO	1	0
9	A	1037	EDO	1	0
9	A	1041	EDO	1	0
11	A	1049	PGE	5	0
11	A	1051	PGE	2	0
8	A	1016	SCN	2	0
8	A	1019	SCN	1	0
9	A	1038	EDO	1	0
9	A	1029	EDO	3	0
9	A	1043	EDO	4	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	862/938 (91%)	-0.01	25 (2%) 51 54	16, 25, 53, 110	0
2	B	8/9 (88%)	2.15	4 (50%) 0 0	43, 47, 58, 79	0
All	All	870/947 (91%)	0.01	29 (3%) 46 49	16, 25, 54, 110	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	559	THR	9.6
1	A	557	PRO	7.6
1	A	112	GLY	6.3
1	A	111	ALA	5.8
1	A	553	SER	5.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	D	4	11/12	0.21	0.47	76,83,89,92	0
4	BMA	D	3	11/12	0.49	0.47	63,77,82,85	0
4	NAG	D	2	14/15	0.62	0.38	51,62,76,94	0
3	NAG	C	3	14/15	0.63	0.24	63,82,88,90	0
3	NAG	C	1	14/15	0.65	0.21	47,61,71,72	0

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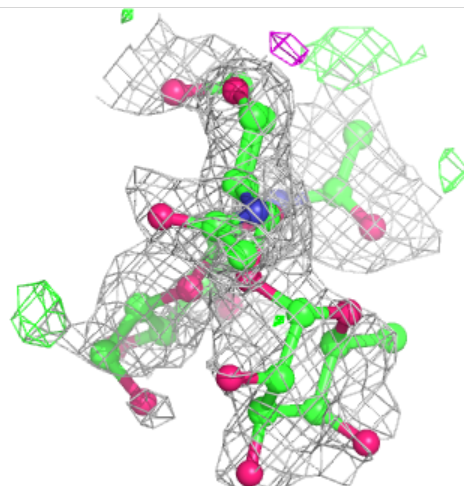
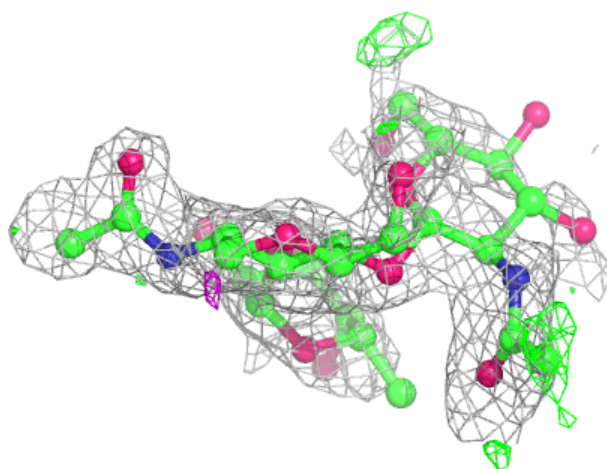
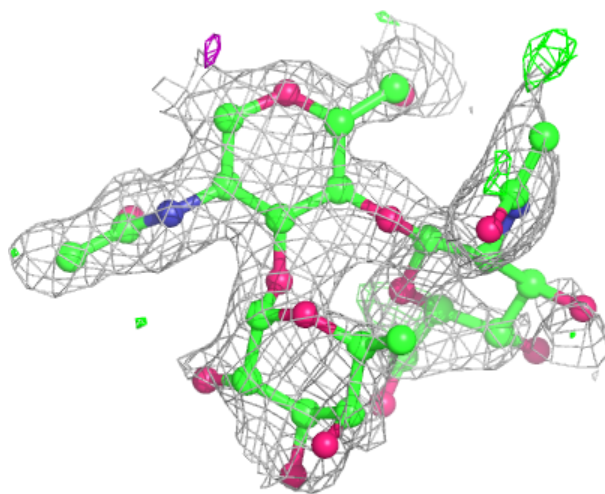
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	E	1	14/15	0.70	0.22	54,63,74,75	0
5	NAG	E	2	14/15	0.72	0.45	78,88,92,93	0
4	NAG	D	1	14/15	0.74	0.17	40,44,54,59	0
3	FUC	C	2	10/11	0.82	0.22	83,90,92,93	0

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.

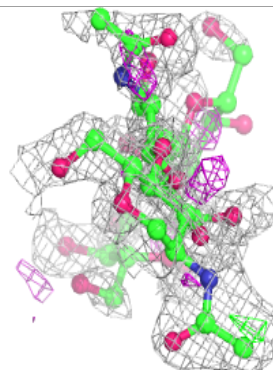
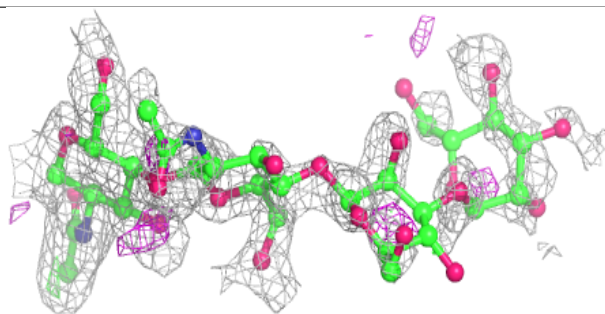
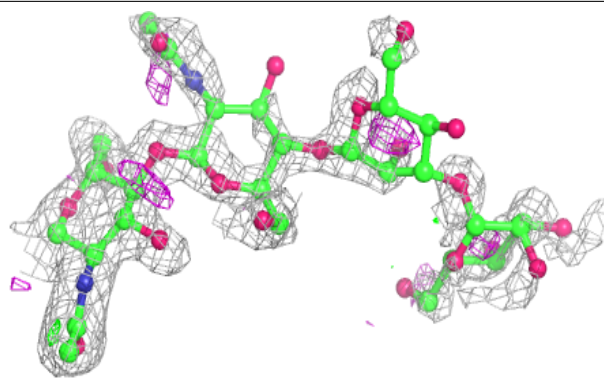
Electron density around Chain C:

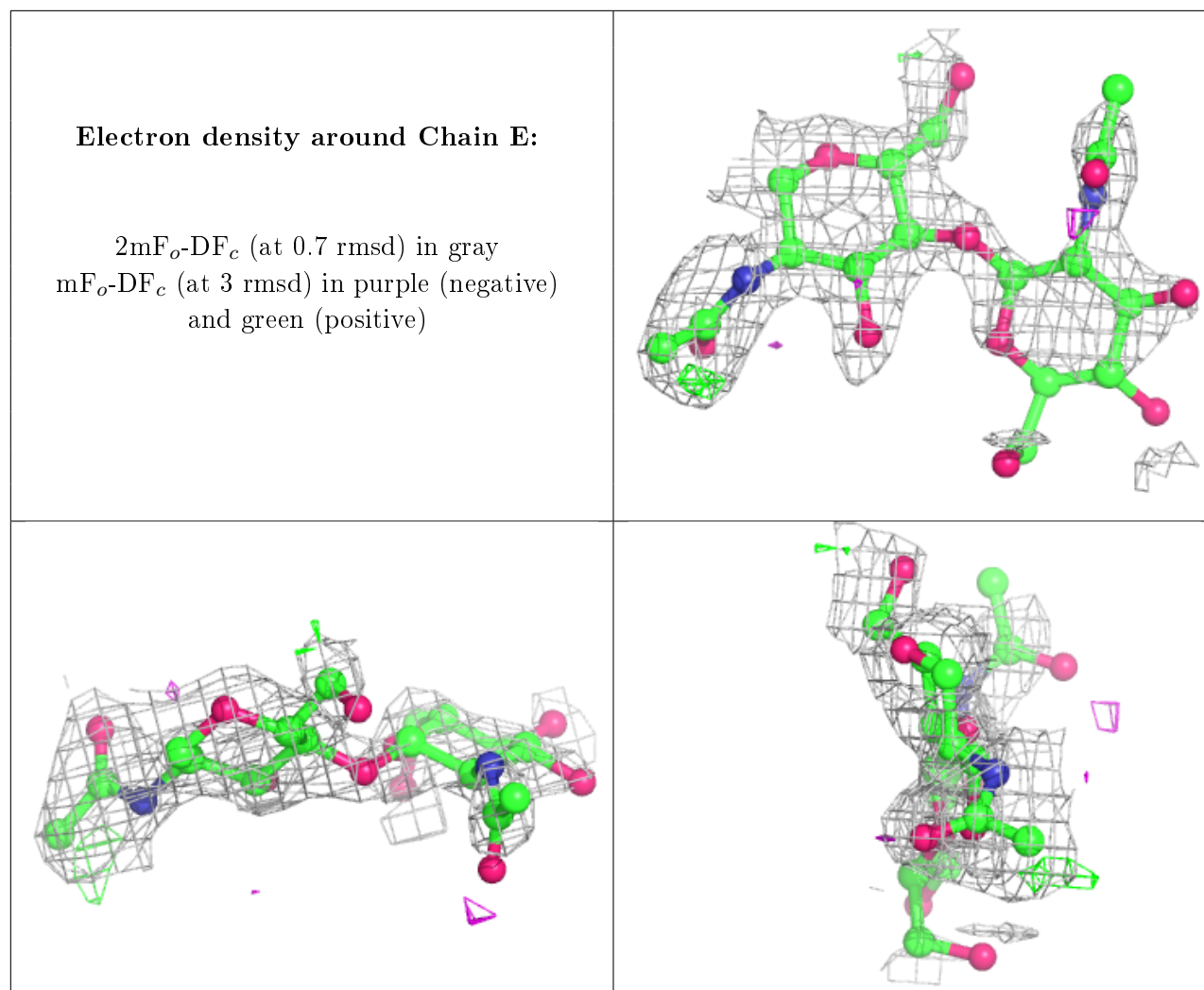
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

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





6.4 Ligands ⓘ

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
9	EDO	A	1038	4/4	0.34	0.28	57,69,75,75	0
8	SCN	A	1015	3/3	0.51	0.20	73,73,75,76	0
8	SCN	A	1020	3/3	0.56	0.21	76,76,79,84	0
8	SCN	A	1021	3/3	0.58	0.18	79,79,83,87	0
6	NAG	A	1010	14/15	0.61	0.38	94,104,108,112	0
11	PGE	A	1050	10/10	0.72	0.32	37,58,79,80	0
9	EDO	A	1033	4/4	0.72	0.20	71,85,88,88	0
9	EDO	A	1040	4/4	0.73	0.15	50,61,69,73	0
9	EDO	A	1044	4/4	0.76	0.50	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	EDO	A	1042	4/4	0.76	0.43	55,67,77,81	0
9	EDO	A	1034	4/4	0.77	0.25	63,76,82,85	0
9	EDO	A	1036	4/4	0.79	0.14	56,68,73,75	0
9	EDO	A	1043	4/4	0.79	0.14	60,73,82,82	0
8	SCN	A	1016	3/3	0.80	0.12	49,49,51,54	0
11	PGE	A	1049	10/10	0.81	0.24	38,71,85,86	0
9	EDO	A	1039	4/4	0.82	0.14	54,65,73,76	0
9	EDO	A	1037	4/4	0.82	0.10	51,61,69,72	0
9	EDO	A	1026	4/4	0.82	0.20	28,39,47,54	0
8	SCN	A	1014	3/3	0.83	0.16	38,38,44,46	0
8	SCN	A	1022	3/3	0.84	0.32	86,86,88,91	0
9	EDO	A	1028	4/4	0.84	0.12	31,40,51,57	0
11	PGE	A	1051	10/10	0.85	0.30	40,74,90,93	0
8	SCN	A	1019	3/3	0.86	0.20	79,79,84,90	0
9	EDO	A	1032	4/4	0.87	0.15	32,48,58,65	0
10	NA	A	1048	1/1	0.87	0.13	50,50,50,50	0
9	EDO	A	1030	4/4	0.87	0.12	45,54,60,63	0
9	EDO	A	1031	4/4	0.88	0.15	33,46,56,68	0
9	EDO	A	1025	4/4	0.88	0.17	26,40,53,53	0
9	EDO	A	1035	4/4	0.90	0.13	44,55,63,66	0
8	SCN	A	1018	3/3	0.90	0.18	59,59,70,77	0
9	EDO	A	1029	4/4	0.92	0.21	39,56,67,67	0
8	SCN	A	1017	3/3	0.92	0.15	50,50,50,58	0
9	EDO	A	1041	4/4	0.93	0.20	19,23,38,45	0
10	NA	A	1047	1/1	0.95	0.08	49,49,49,49	0
10	NA	A	1045	1/1	0.95	0.08	38,38,38,38	0
9	EDO	A	1023	4/4	0.95	0.18	21,47,57,57	0
9	EDO	A	1024	4/4	0.96	0.11	24,29,34,35	0
10	NA	A	1046	1/1	0.96	0.07	39,39,39,39	0
8	SCN	A	1012	3/3	0.97	0.12	23,23,30,37	0
8	SCN	A	1013	3/3	0.97	0.14	33,33,36,38	0
9	EDO	A	1027	4/4	0.98	0.08	27,32,38,44	0
7	ZN	A	1011	1/1	1.00	0.10	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.