



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:08 AM UTC

PDB ID : 8I5P / pdb_00008i5p
Title : Crystal structure of TxGH116 D593A acid/base mutant from Thermoanaerobacterium xylanolyticum with cellobiose
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Deposited on : 2023-01-26
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

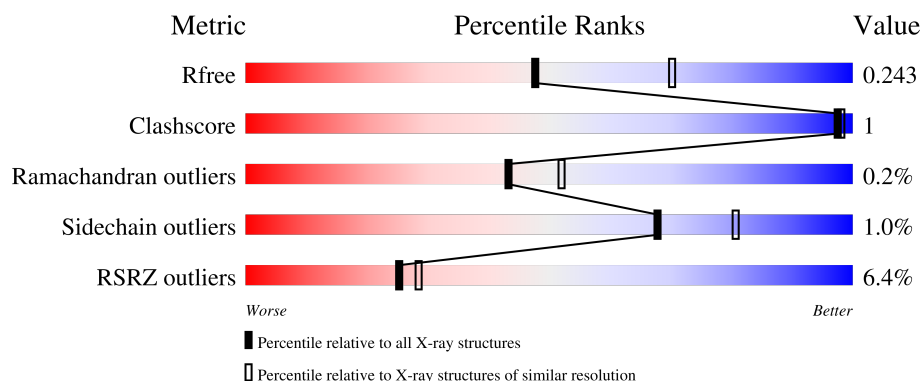
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	799	2% 93% • •
1	B	799	10% 94% • •
2	D	2	50% 50%
2	E	2	50% 50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12615 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-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	769	Total	C	N	O	S	0	4	0
			6192	3997	993	1174	28			
1	B	769	Total	C	N	O	S	0	3	0
			6054	3915	965	1146	28			

There are 24 discrepancies between the modelled and reference sequences:

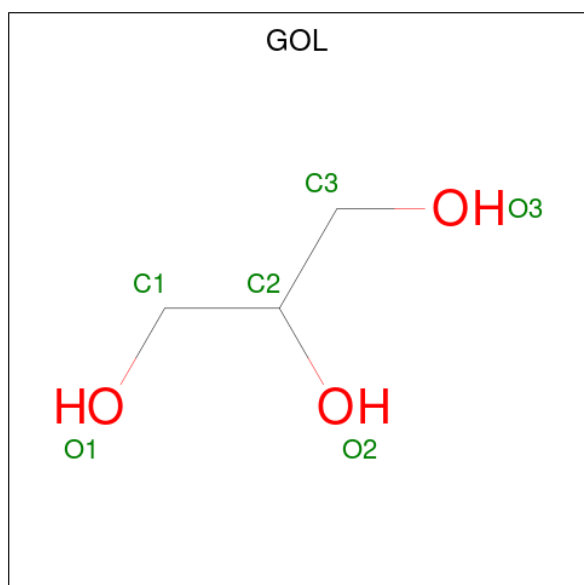
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ALA	-	expression tag	UNP F6BL85
A	17	MET	-	expression tag	UNP F6BL85
A	18	ALA	-	expression tag	UNP F6BL85
A	593	ALA	ASP	engineered mutation	UNP F6BL85
A	807	LEU	-	expression tag	UNP F6BL85
A	808	GLU	-	expression tag	UNP F6BL85
A	809	HIS	-	expression tag	UNP F6BL85
A	810	HIS	-	expression tag	UNP F6BL85
A	811	HIS	-	expression tag	UNP F6BL85
A	812	HIS	-	expression tag	UNP F6BL85
A	813	HIS	-	expression tag	UNP F6BL85
A	814	HIS	-	expression tag	UNP F6BL85
B	16	ALA	-	expression tag	UNP F6BL85
B	17	MET	-	expression tag	UNP F6BL85
B	18	ALA	-	expression tag	UNP F6BL85
B	593	ALA	ASP	engineered mutation	UNP F6BL85
B	807	LEU	-	expression tag	UNP F6BL85
B	808	GLU	-	expression tag	UNP F6BL85
B	809	HIS	-	expression tag	UNP F6BL85
B	810	HIS	-	expression tag	UNP F6BL85
B	811	HIS	-	expression tag	UNP F6BL85
B	812	HIS	-	expression tag	UNP F6BL85
B	813	HIS	-	expression tag	UNP F6BL85
B	814	HIS	-	expression tag	UNP F6BL85

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



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

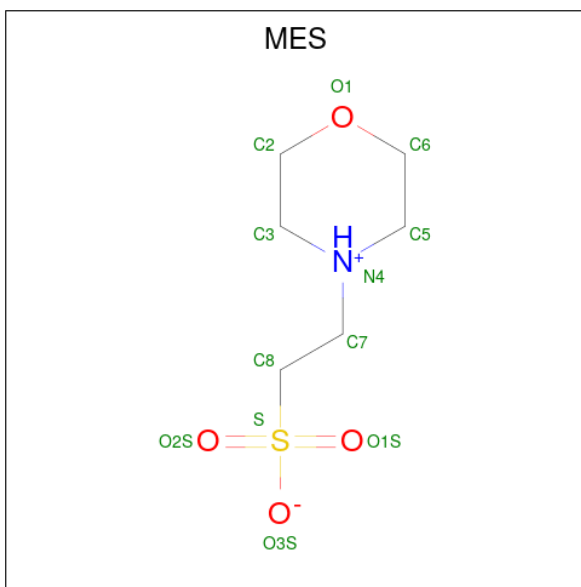


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

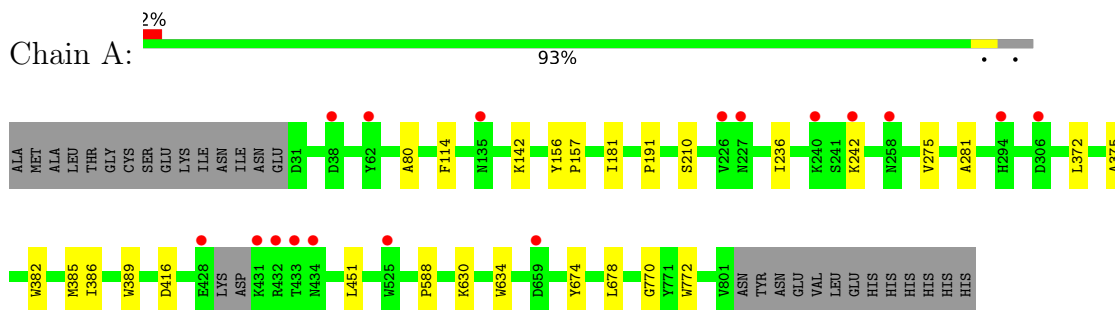
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	189	Total	O	0	0
			189	189		
6	B	114	Total	O	0	0
			114	114		

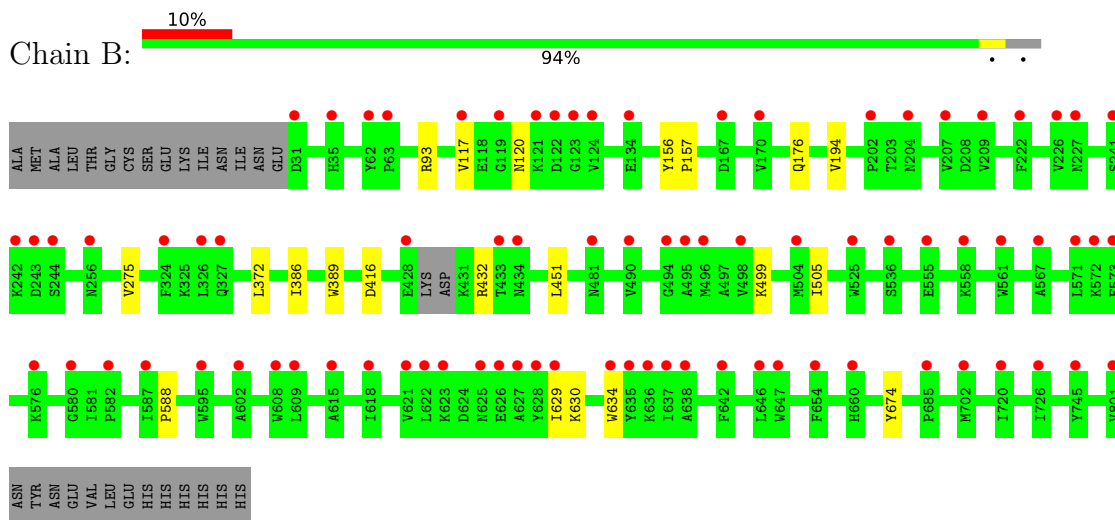
3 Residue-property plots [i](#)

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-glucosidase



- Molecule 1: beta-glucosidase



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



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.07Å 100.50Å 173.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.35 40.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.35) 99.9 (40.00-2.35)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.190 , 0.241 0.196 , 0.243	Depositor DCC
R_{free} test set	3529 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12615	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: CA, MES, GOL, BGC

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	0.57	0/6373	0.80	0/8655
1	B	0.58	0/6233	0.82	0/8488
All	All	0.57	0/12606	0.81	0/17143

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	6192	0	5845	10	0
1	B	6054	0	5600	9	0
2	D	23	0	21	0	0
2	E	23	0	21	0	0
3	A	6	0	8	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	12	0	13	0	0
6	A	189	0	0	0	0
6	B	114	0	0	0	0
All	All	12615	0	11508	19	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 1.

All (19) 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:451:LEU:HD22	1:B:505:ILE:HG21	1.78	0.65
1:A:630:LYS:HE2	1:A:634:TRP:CZ2	2.35	0.61
1:B:93:ARG:NH2	1:B:416:ASP:OD2	2.38	0.56
1:B:386:ILE:HA	1:B:389[A]:TRP:CD1	2.49	0.48
1:B:630:LYS:HE2	1:B:634:TRP:CZ2	2.48	0.48
1:A:80:ALA:HB1	1:A:191:PRO:HB3	1.96	0.47
1:A:181:ILE:HG21	1:A:385:MET:HE2	1.97	0.47
1:B:117:VAL:HB	1:B:120:ASN:OD1	2.16	0.45
1:B:389[B]:TRP:CD1	1:B:389[B]:TRP:C	2.95	0.45
1:A:156:TYR:CD1	1:A:157:PRO:HA	2.53	0.44
1:A:386:ILE:HA	1:A:389[A]:TRP:CD1	2.53	0.44
1:B:156:TYR:CD1	1:B:157:PRO:HA	2.53	0.43
1:A:236:ILE:HG12	1:A:281:ALA:HB2	2.00	0.43
1:A:389[B]:TRP:CD1	1:A:389[B]:TRP:C	2.95	0.43
1:B:389[B]:TRP:CD1	1:B:389[B]:TRP:O	2.71	0.43
1:A:114:PHE:HB3	1:A:210:SER:HB2	2.02	0.41
1:A:770:GLY:HA2	1:A:772:TRP:CZ3	2.56	0.41
1:B:176:GLN:HA	1:B:194:VAL:O	2.21	0.40
1:A:375:ALA:HA	1:A:382:TRP:CH2	2.56	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	769/799 (96%)	741 (96%)	26 (3%)	2 (0%)	36	43
1	B	768/799 (96%)	739 (96%)	28 (4%)	1 (0%)	48	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1537/1598 (96%)	1480 (96%)	54 (4%)	3 (0%)	43 52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	588	PRO
1	A	242	LYS
1	A	588	PRO

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	642/684 (94%)	635 (99%)	7 (1%)	65 79
1	B	608/684 (89%)	602 (99%)	6 (1%)	68 81
All	All	1250/1368 (91%)	1237 (99%)	13 (1%)	68 81

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	LYS
1	A	275	VAL
1	A	372	LEU
1	A	416	ASP
1	A	451	LEU
1	A	674	TYR
1	A	678	LEU
1	B	275	VAL
1	B	372	LEU
1	B	432	ARG
1	B	499	LYS
1	B	629	ILE
1	B	674	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	ASN
1	A	690	GLN
1	A	729	GLN
1	B	216	GLN
1	B	367	ASN
1	B	584	ASN
1	B	616	GLN
1	B	690	GLN
1	B	729	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 ⓘ

4 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	D	1	2	12,12,12	0.48	0	17,17,17	0.84	0
2	BGC	D	2	2	11,11,12	0.35	0	15,15,17	1.08	1 (6%)
2	BGC	E	1	2	12,12,12	0.50	0	17,17,17	0.91	0
2	BGC	E	2	2	11,11,12	0.35	0	15,15,17	1.25	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	BGC	D	1	2	-	0/2/22/22	0/1/1/1
2	BGC	D	2	2	-	0/2/19/22	0/1/1/1
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	E	2	BGC	C1-C2-C3	2.87	113.83	109.64
2	D	2	BGC	C1-C2-C3	2.86	113.81	109.64

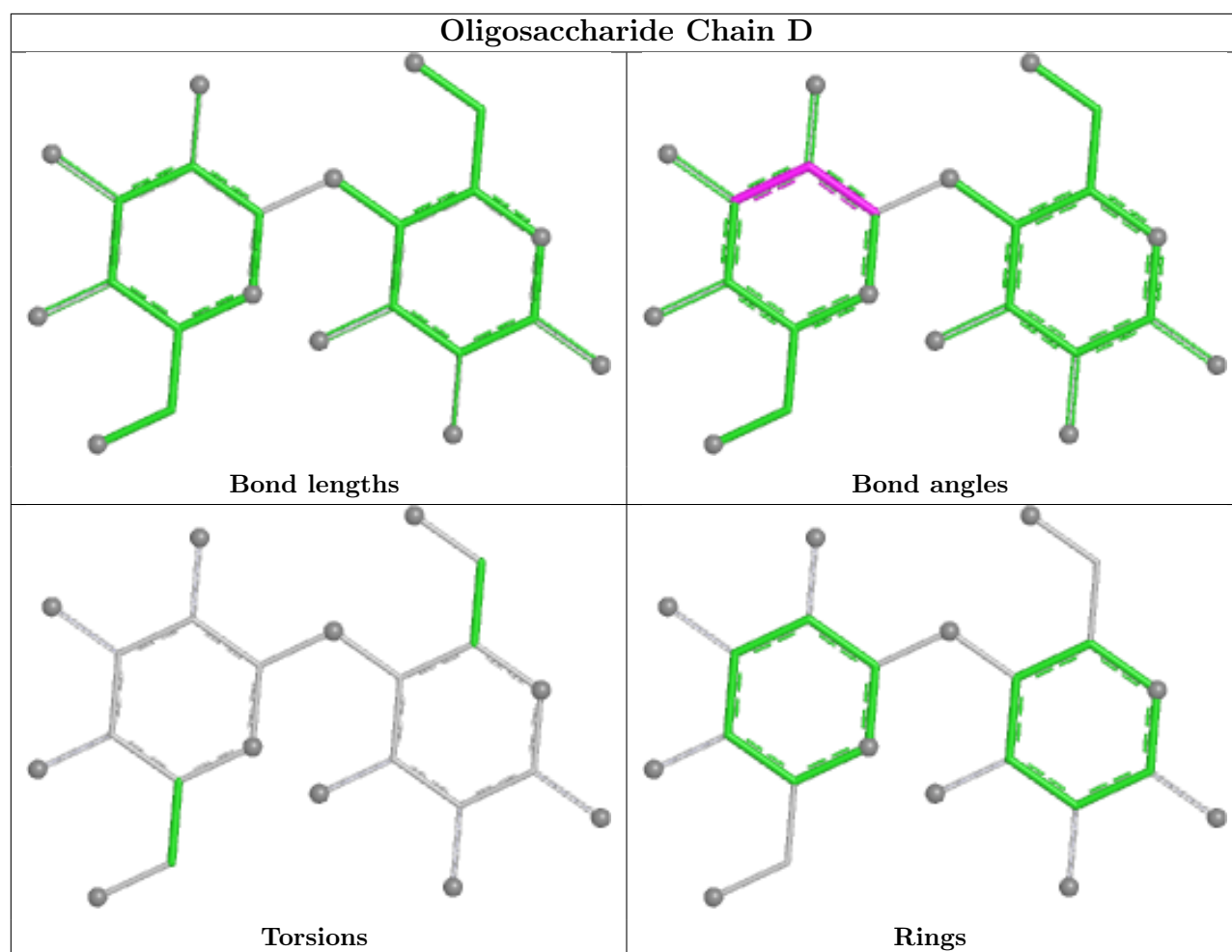
There are no chirality outliers.

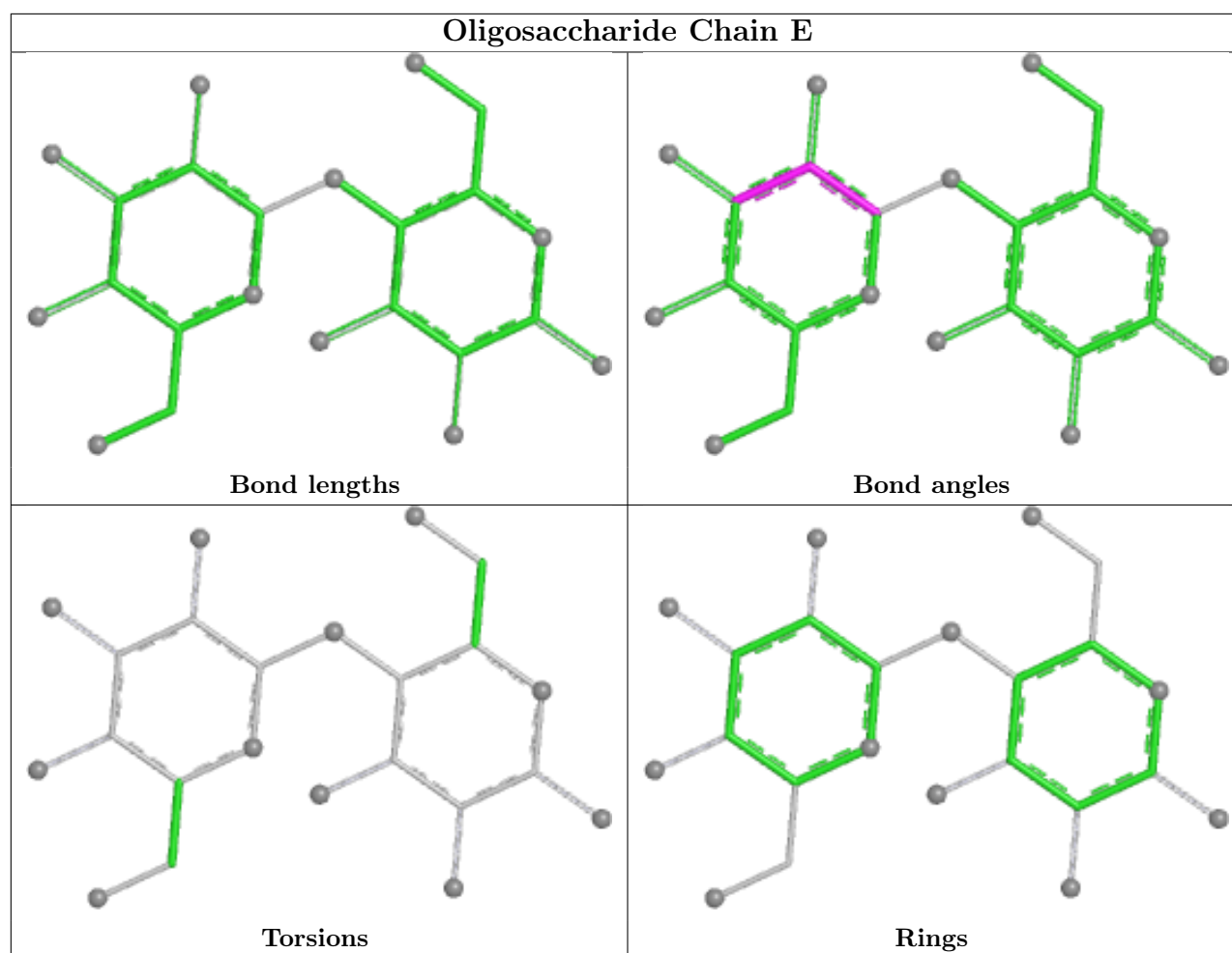
There are no torsion outliers.

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
5	MES	A	1003	-	12,12,12	2.42	1 (8%)	15,16,16	1.47	2 (13%)
3	GOL	A	1001	-	5,5,5	0.37	0	5,5,5	0.46	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	MES	A	1003	-	-	5/6/14/14	0/1/1/1
3	GOL	A	1001	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1003	MES	C8-S	-7.99	1.66	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1003	MES	O1S-S-C8	4.15	113.00	106.73
5	A	1003	MES	O2S-S-C8	2.22	110.08	106.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1003	MES	C7-C8-S-O3S
5	A	1003	MES	C8-C7-N4-C5
5	A	1003	MES	C7-C8-S-O1S
5	A	1003	MES	C7-C8-S-O2S
5	A	1003	MES	C8-C7-N4-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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	769/799 (96%)	-0.18	17 (2%) 62 67	14, 34, 55, 98	4 (0%)
1	B	769/799 (96%)	0.60	81 (10%) 11 13	18, 47, 82, 105	3 (0%)
All	All	1538/1598 (96%)	0.21	98 (6%) 25 28	14, 39, 74, 105	7 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	ASP	5.6
1	B	204	ASN	4.2
1	B	433	THR	4.2
1	B	117	VAL	4.2
1	B	745	TYR	4.2
1	B	226	VAL	4.0
1	A	433	THR	3.9
1	A	431	LYS	3.6
1	B	622	LEU	3.5
1	B	623	LYS	3.5
1	B	628	TYR	3.4
1	B	207	VAL	3.3
1	B	627	ALA	3.3
1	B	629	ILE	3.2
1	B	428	GLU	3.2
1	A	226	VAL	3.1
1	B	243	ASP	3.1
1	B	525	TRP	3.1
1	B	801	VAL	3.1
1	B	587	ILE	3.1
1	B	327	GLN	3.1
1	B	326	LEU	3.1
1	B	634	TRP	3.0
1	B	646	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	595	TRP	2.9
1	B	567	ALA	2.8
1	A	525	TRP	2.8
1	B	660	HIS	2.8
1	B	636	LYS	2.8
1	B	635	TYR	2.7
1	B	121	LYS	2.7
1	B	490	VAL	2.7
1	A	62	TYR	2.6
1	B	167	ASP	2.6
1	B	209	VAL	2.6
1	B	571	LEU	2.6
1	A	434	ASN	2.6
1	B	608	TRP	2.6
1	B	498	VAL	2.6
1	B	555	GLU	2.5
1	B	573	GLU	2.5
1	B	625	ASN	2.5
1	B	576	LYS	2.5
1	B	242	LYS	2.5
1	B	119	GLY	2.5
1	B	62	TYR	2.5
1	B	170	VAL	2.4
1	A	38	ASP	2.4
1	A	258	ASN	2.4
1	B	123	GLY	2.4
1	B	638	ALA	2.4
1	B	324	PHE	2.4
1	B	621	VAL	2.4
1	B	642	PHE	2.4
1	B	496	MET	2.4
1	B	256	ASN	2.4
1	B	626	GLU	2.4
1	B	227	ASN	2.3
1	B	647	TRP	2.3
1	B	654	PHE	2.3
1	B	561	TRP	2.3
1	B	702[A]	MET	2.3
1	A	240	LYS	2.3
1	A	227	ASN	2.2
1	B	504	MET	2.2
1	B	615	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	244[A]	SER	2.2
1	B	720	ILE	2.2
1	B	609	LEU	2.2
1	A	135	ASN	2.2
1	A	306	ASP	2.2
1	A	432	ARG	2.2
1	B	685	PRO	2.2
1	B	558	LYS	2.2
1	B	222	PHE	2.2
1	A	242	LYS	2.2
1	B	35	HIS	2.2
1	A	428	GLU	2.1
1	B	31	ASP	2.1
1	B	124	VAL	2.1
1	B	582	PRO	2.1
1	B	494	GLY	2.1
1	B	241	SER	2.1
1	B	434	ASN	2.1
1	B	637	ILE	2.1
1	B	580	GLY	2.1
1	B	536	SER	2.1
1	B	602	ALA	2.1
1	A	294	HIS	2.1
1	B	726	ILE	2.1
1	B	202	PRO	2.1
1	B	572	LYS	2.0
1	A	659	ASP	2.0
1	B	481	ASN	2.0
1	B	618	ILE	2.0
1	B	63	PRO	2.0
1	B	134	GLU	2.0
1	B	495	ALA	2.0

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

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

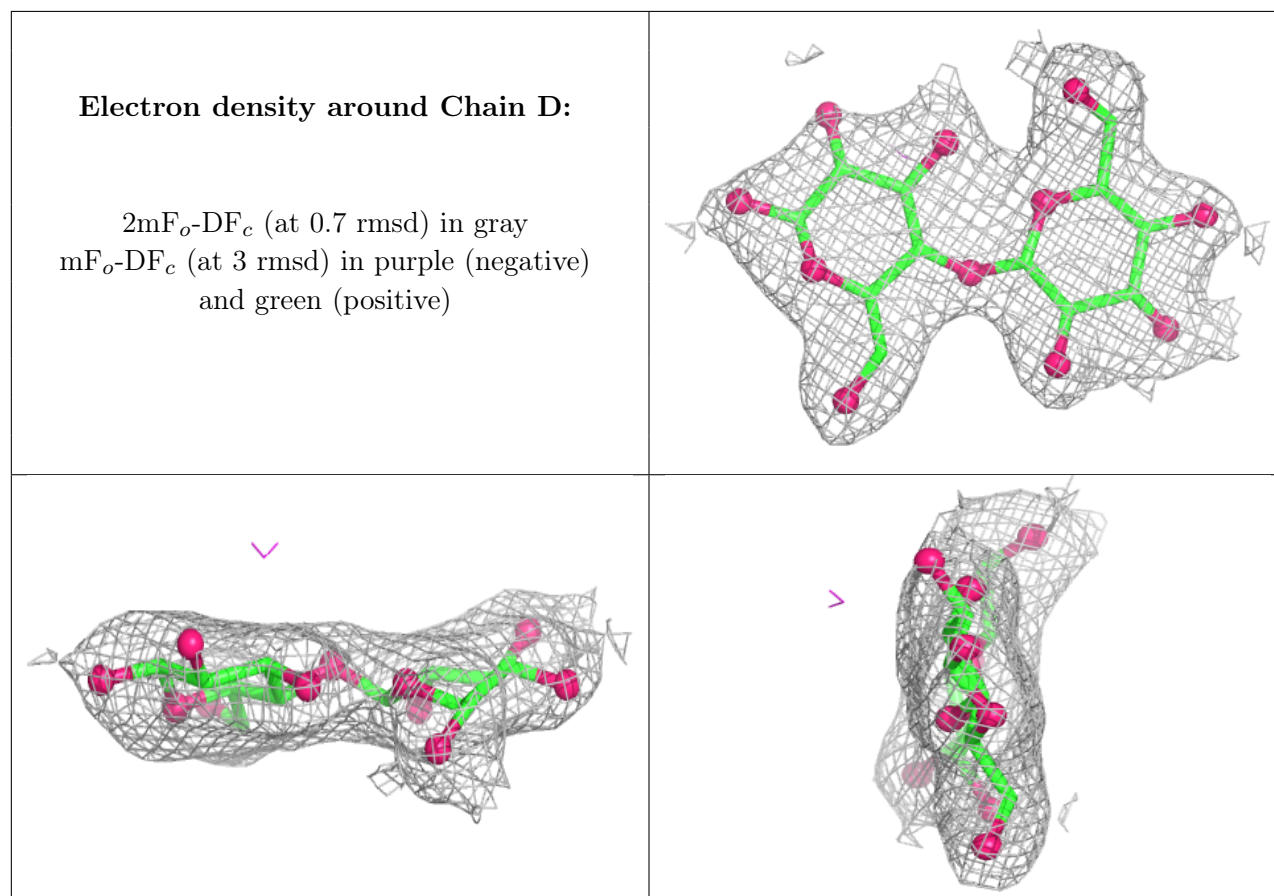
6.3 Carbohydrates [i](#)

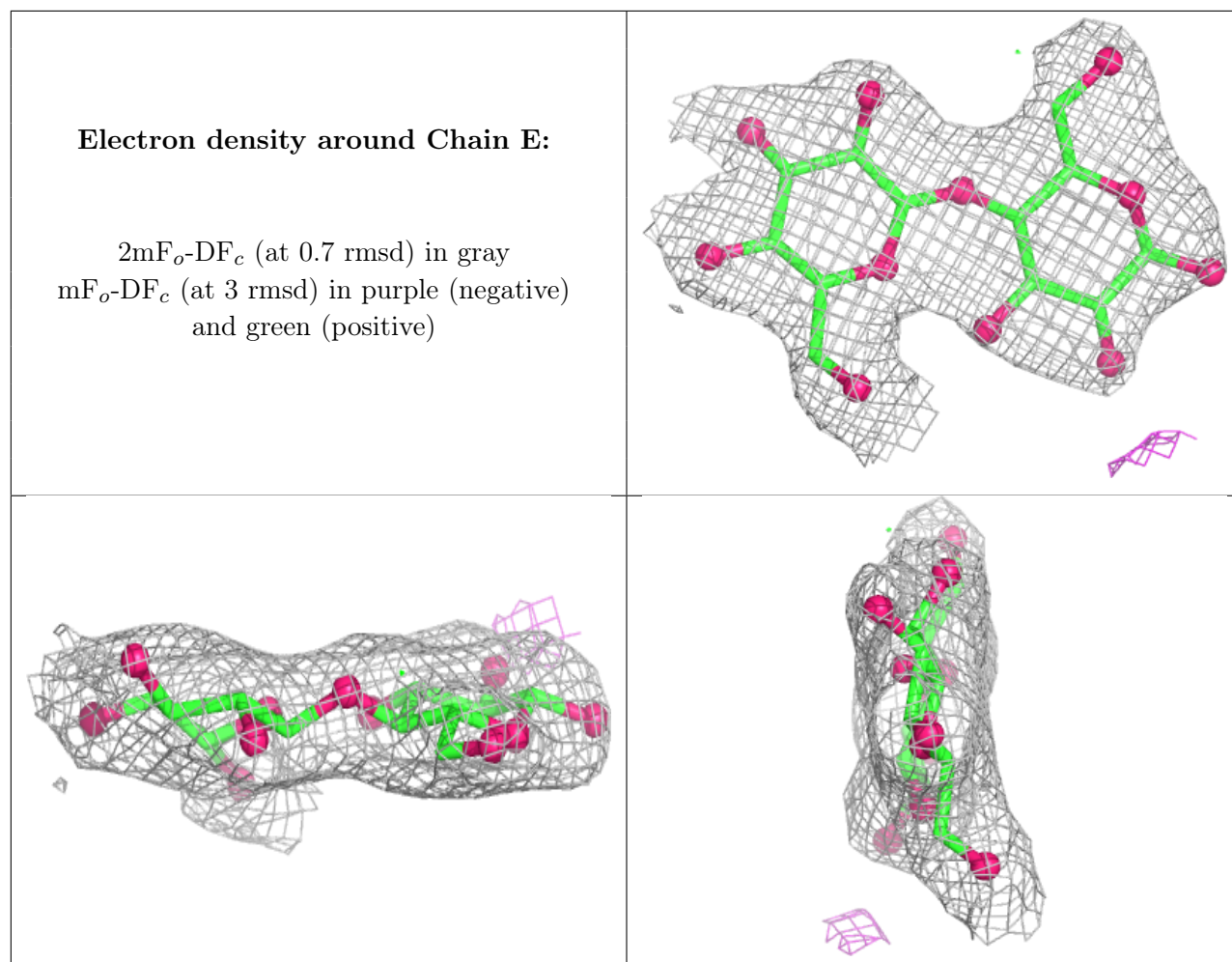
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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
2	BGC	D	1	12/12	0.85	0.11	38,39,46,46	0
2	BGC	D	2	11/12	0.93	0.07	33,34,35,36	0
2	BGC	E	1	12/12	-	-	51,56,58,59	0
2	BGC	E	2	11/12	-	-	41,44,47,48	0

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	1001	6/6	0.89	0.11	44,48,51,56	0
4	CA	B	901	1/1	0.95	0.05	75,75,75,75	0
5	MES	A	1003	12/12	0.96	0.08	35,37,38,39	0
4	CA	A	1002	1/1	0.97	0.05	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.