



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 12:24 pm BST

PDB ID : 6F91
Title : Structure of the family GH92 alpha-mannosidase BT3965 from *Bacteroides thetaiotaomicron*
Authors : Thompson, A.J.; Spears, R.J.; Zhu, Y.; Suits, M.D.L.; Williams, S.J.; Gilbert, H.J.; Davies, G.J.
Deposited on : 2017-12-13
Resolution : 1.80 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 : 2.11
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) : 2.11

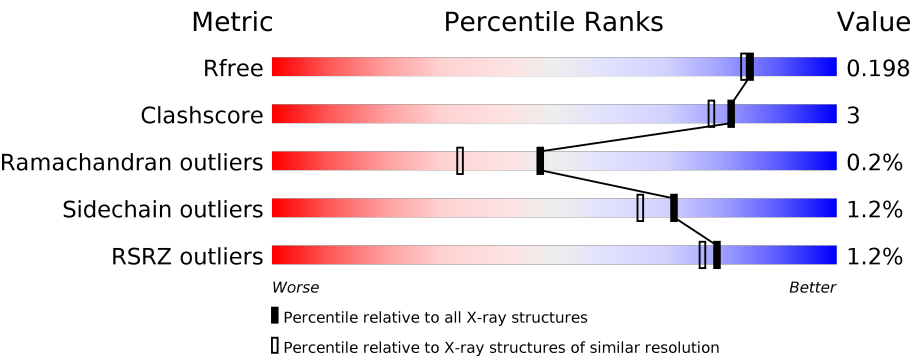
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	764	<div><div>2%</div><div><div></div><div>90%</div><div>7%</div><div>••</div></div></div>
1	B	764	<div><div>%</div><div><div></div><div>90%</div><div>7%</div><div>•</div></div></div>
1	C	764	<div><div>%</div><div><div></div><div>91%</div><div>6%</div><div>•</div></div></div>
1	D	764	<div><div>%</div><div><div></div><div>90%</div><div>7%</div><div>••</div></div></div>
1	E	764	<div><div>%</div><div><div></div><div>90%</div><div>7%</div><div>••</div></div></div>
1	F	764	<div><div>3%</div><div><div></div><div>91%</div><div>5%</div><div>•</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	764	<div><div>%</div><div><div></div></div><div>88%</div><div>8%</div><div>• •</div></div>
1	H	764	<div><div>%</div><div><div></div></div><div>90%</div><div>6%</div><div>• •</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 55039 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 Putative alpha-1,2-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	740	Total	C	N	O	S	0	10	0
			6002	3840	986	1140	36			
1	B	738	Total	C	N	O	S	0	13	0
			5971	3827	973	1134	37			
1	C	747	Total	C	N	O	S	0	15	0
			6052	3881	990	1146	35			
1	D	742	Total	C	N	O	S	0	17	0
			6061	3886	1002	1138	35			
1	E	742	Total	C	N	O	S	0	22	0
			6086	3902	1000	1150	34			
1	F	736	Total	C	N	O	S	0	6	0
			5893	3772	970	1117	34			
1	G	742	Total	C	N	O	S	0	10	0
			6025	3858	996	1136	35			
1	H	741	Total	C	N	O	S	0	14	0
			6049	3871	1001	1140	37			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	757	LEU	-	expression tag	UNP A0A139JT15
A	758	GLU	-	expression tag	UNP A0A139JT15
A	759	HIS	-	expression tag	UNP A0A139JT15
A	760	HIS	-	expression tag	UNP A0A139JT15
A	761	HIS	-	expression tag	UNP A0A139JT15
A	762	HIS	-	expression tag	UNP A0A139JT15
A	763	HIS	-	expression tag	UNP A0A139JT15
A	764	HIS	-	expression tag	UNP A0A139JT15
B	757	LEU	-	expression tag	UNP A0A139JT15
B	758	GLU	-	expression tag	UNP A0A139JT15
B	759	HIS	-	expression tag	UNP A0A139JT15
B	760	HIS	-	expression tag	UNP A0A139JT15
B	761	HIS	-	expression tag	UNP A0A139JT15

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Chain	Residue	Modelled	Actual	Comment	Reference
B	762	HIS	-	expression tag	UNP A0A139JT15
B	763	HIS	-	expression tag	UNP A0A139JT15
B	764	HIS	-	expression tag	UNP A0A139JT15
C	757	LEU	-	expression tag	UNP A0A139JT15
C	758	GLU	-	expression tag	UNP A0A139JT15
C	759	HIS	-	expression tag	UNP A0A139JT15
C	760	HIS	-	expression tag	UNP A0A139JT15
C	761	HIS	-	expression tag	UNP A0A139JT15
C	762	HIS	-	expression tag	UNP A0A139JT15
C	763	HIS	-	expression tag	UNP A0A139JT15
C	764	HIS	-	expression tag	UNP A0A139JT15
D	757	LEU	-	expression tag	UNP A0A139JT15
D	758	GLU	-	expression tag	UNP A0A139JT15
D	759	HIS	-	expression tag	UNP A0A139JT15
D	760	HIS	-	expression tag	UNP A0A139JT15
D	761	HIS	-	expression tag	UNP A0A139JT15
D	762	HIS	-	expression tag	UNP A0A139JT15
D	763	HIS	-	expression tag	UNP A0A139JT15
D	764	HIS	-	expression tag	UNP A0A139JT15
E	757	LEU	-	expression tag	UNP A0A139JT15
E	758	GLU	-	expression tag	UNP A0A139JT15
E	759	HIS	-	expression tag	UNP A0A139JT15
E	760	HIS	-	expression tag	UNP A0A139JT15
E	761	HIS	-	expression tag	UNP A0A139JT15
E	762	HIS	-	expression tag	UNP A0A139JT15
E	763	HIS	-	expression tag	UNP A0A139JT15
E	764	HIS	-	expression tag	UNP A0A139JT15
F	757	LEU	-	expression tag	UNP A0A139JT15
F	758	GLU	-	expression tag	UNP A0A139JT15
F	759	HIS	-	expression tag	UNP A0A139JT15
F	760	HIS	-	expression tag	UNP A0A139JT15
F	761	HIS	-	expression tag	UNP A0A139JT15
F	762	HIS	-	expression tag	UNP A0A139JT15
F	763	HIS	-	expression tag	UNP A0A139JT15
F	764	HIS	-	expression tag	UNP A0A139JT15
G	757	LEU	-	expression tag	UNP A0A139JT15
G	758	GLU	-	expression tag	UNP A0A139JT15
G	759	HIS	-	expression tag	UNP A0A139JT15
G	760	HIS	-	expression tag	UNP A0A139JT15
G	761	HIS	-	expression tag	UNP A0A139JT15
G	762	HIS	-	expression tag	UNP A0A139JT15
G	763	HIS	-	expression tag	UNP A0A139JT15

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Chain	Residue	Modelled	Actual	Comment	Reference
G	764	HIS	-	expression tag	UNP A0A139JT15
H	757	LEU	-	expression tag	UNP A0A139JT15
H	758	GLU	-	expression tag	UNP A0A139JT15
H	759	HIS	-	expression tag	UNP A0A139JT15
H	760	HIS	-	expression tag	UNP A0A139JT15
H	761	HIS	-	expression tag	UNP A0A139JT15
H	762	HIS	-	expression tag	UNP A0A139JT15
H	763	HIS	-	expression tag	UNP A0A139JT15
H	764	HIS	-	expression tag	UNP A0A139JT15

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	H	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0
3	F	1	Total 1	Ca 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0
4	E	1	Total 1	Cl 1	0	0
4	H	1	Total 1	Cl 1	0	0
4	B	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0
4	A	1	Total 1	Cl 1	0	0
4	F	1	Total 1	Cl 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	776	Total O 776 776	0	0
6	B	891	Total O 892 892	0	1
6	C	979	Total O 979 979	0	0
6	D	885	Total O 885 885	0	0
6	E	943	Total O 947 947	0	4
6	F	537	Total O 537 537	0	0
6	G	899	Total O 904 904	0	5

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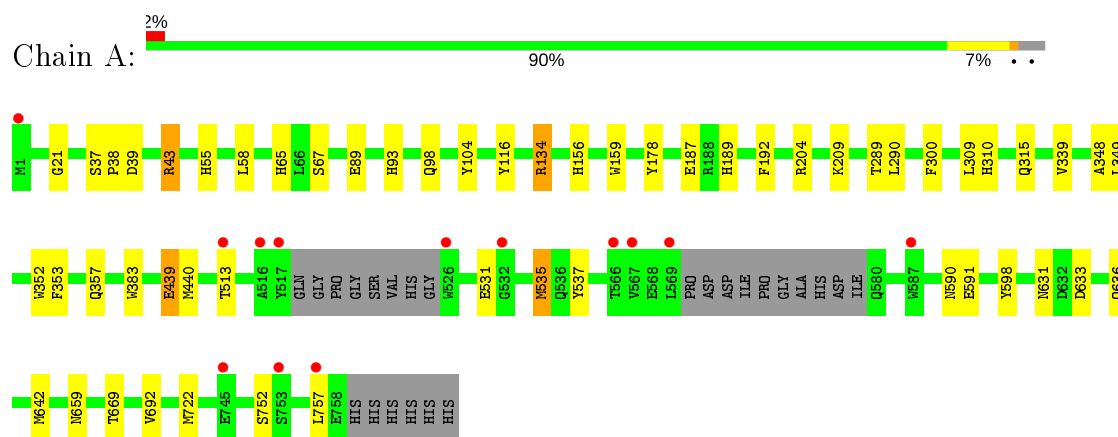
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	849	Total	O	0	3
			852	852		

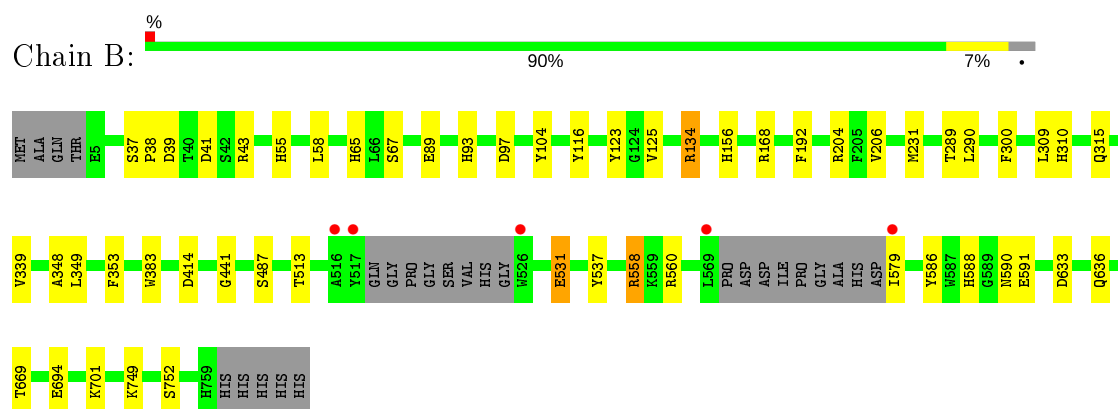
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

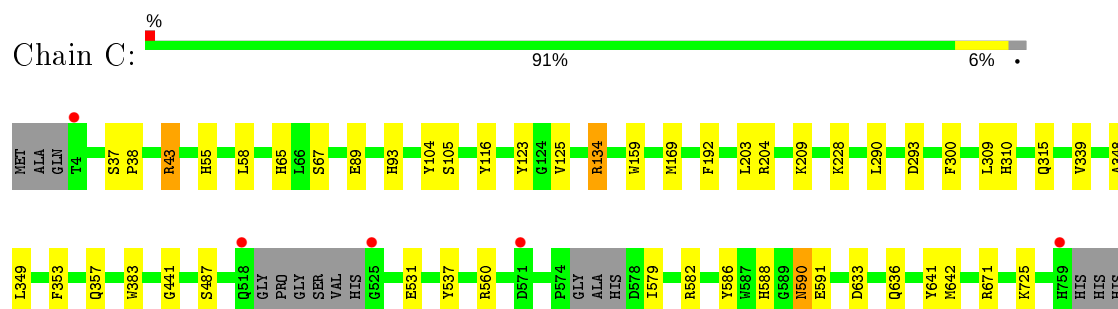
- Molecule 1: Putative alpha-1,2-mannosidase



- Molecule 1: Putative alpha-1,2-mannosidase

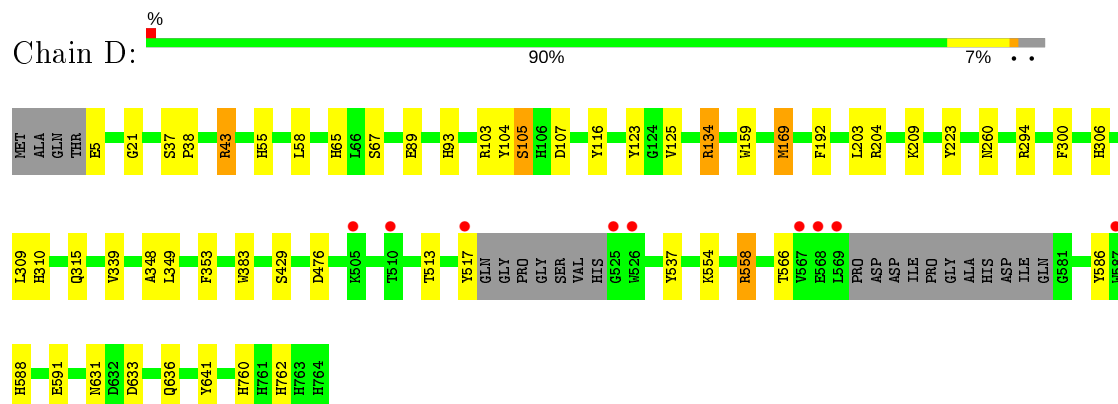


- Molecule 1: Putative alpha-1,2-mannosidase

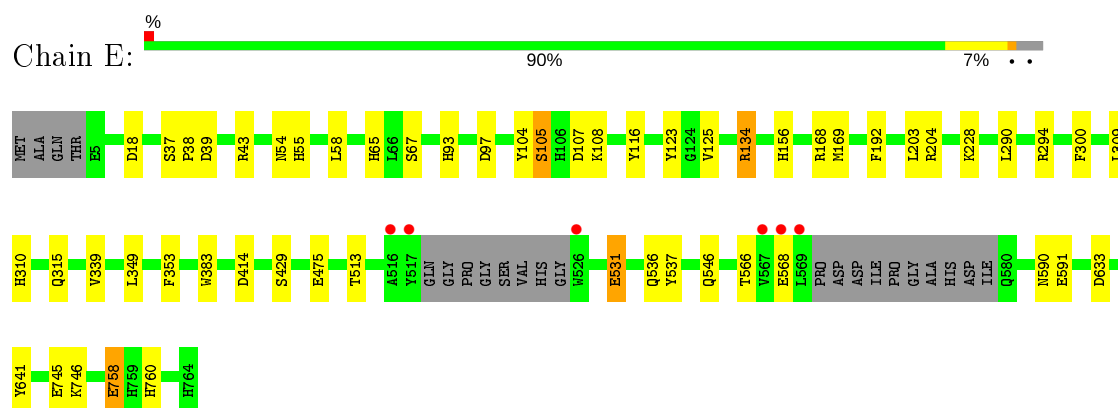


HIS
HIS

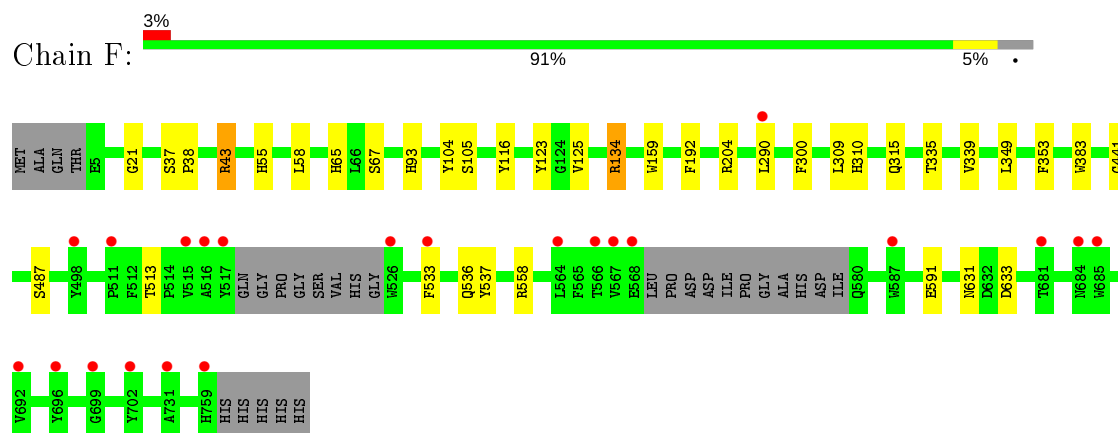
- Molecule 1: Putative alpha-1,2-mannosidase



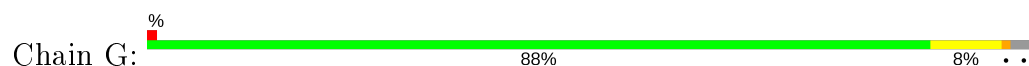
- Molecule 1: Putative alpha-1,2-mannosidase

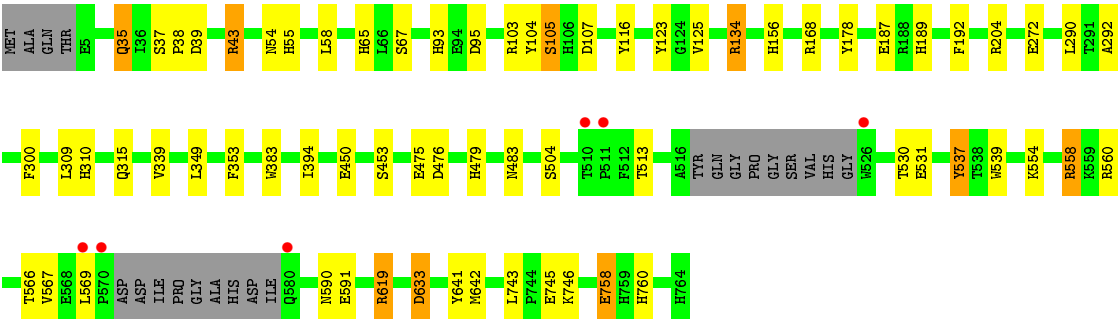


- Molecule 1: Putative alpha-1,2-mannosidase

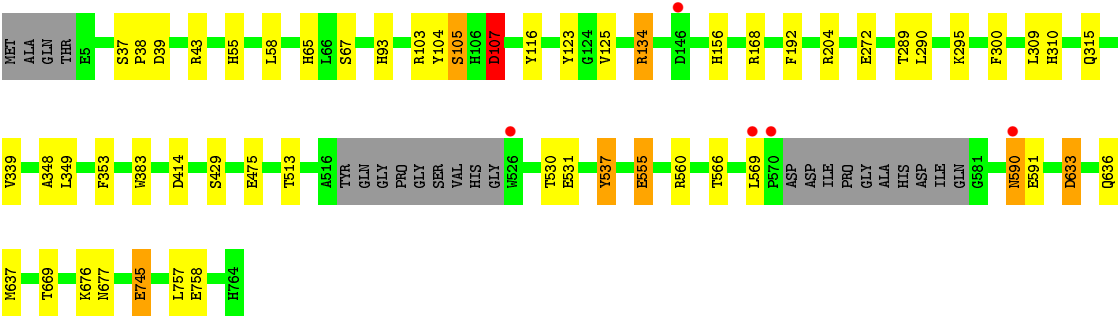
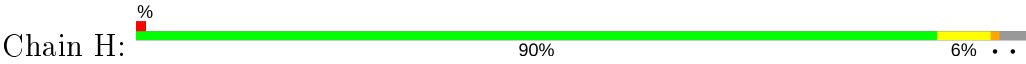


- Molecule 1: Putative alpha-1,2-mannosidase





● Molecule 1: Putative alpha-1,2-mannosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.92Å 184.54Å 183.66Å 90.00° 90.80° 90.00°	Depositor
Resolution (Å)	48.08 – 1.80 48.08 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.08-1.80) 99.5 (48.08-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.160 , 0.185 0.173 , 0.198	Depositor DCC
R_{free} test set	33861 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for -h,-l,-k 0.018 for -h,l,k 0.106 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	55039	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, EDO, CL

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	0.62	1/6199 (0.0%)	0.78	7/8408 (0.1%)
1	B	0.64	2/6180 (0.0%)	0.78	11/8385 (0.1%)
1	C	0.68	0/6269	0.79	6/8508 (0.1%)
1	D	0.67	1/6290 (0.0%)	0.81	13/8528 (0.2%)
1	E	0.66	0/6321	0.80	10/8575 (0.1%)
1	F	0.57	0/6080	0.75	4/8256 (0.0%)
1	G	0.65	2/6227 (0.0%)	0.81	12/8441 (0.1%)
1	H	0.66	5/6260 (0.1%)	0.85	19/8488 (0.2%)
All	All	0.65	11/49826 (0.0%)	0.80	82/67589 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	G	0	1
1	H	0	1
All	All	0	3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	272	GLU	CD-OE2	8.44	1.34	1.25
1	H	555	GLU	CD-OE2	6.20	1.32	1.25
1	H	758	GLU	CD-OE2	-5.58	1.19	1.25
1	G	504	SER	CB-OG	-5.51	1.35	1.42
1	D	105	SER	CB-OG	-5.42	1.35	1.42

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	43[A]	ARG	NE-CZ-NH2	11.66	126.13	120.30
1	H	43[B]	ARG	NE-CZ-NH2	11.66	126.13	120.30
1	C	134	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	H	134	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	D	134	ARG	NE-CZ-NH1	8.35	124.48	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	745[A]	GLU	Peptide
1	G	745	GLU	Peptide
1	H	745[A]	GLU	Peptide

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	6002	0	5675	35	0
1	B	5971	0	5646	25	0
1	C	6052	0	5743	27	0
1	D	6061	0	5757	33	0
1	E	6086	0	5767	31	0
1	F	5893	0	5527	18	0
1	G	6025	0	5707	54	0
1	H	6049	0	5724	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	12	0	18	1	0
5	B	12	0	18	0	0
5	C	12	0	18	0	0
5	D	20	0	30	2	0
5	E	12	0	18	0	0
5	F	8	0	12	0	0
5	G	16	0	24	2	0
5	H	12	0	18	0	0
6	A	776	0	0	3	2
6	B	892	0	0	5	1
6	C	979	0	0	3	3
6	D	885	0	0	7	3
6	E	947	0	0	11	1
6	F	537	0	0	2	0
6	G	904	0	0	14	0
6	H	852	0	0	4	2
All	All	55039	0	45702	248	6

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.

The worst 5 of 248 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:G:642[B]:MET:HA	1:G:642[B]:MET:CE	1.63	1.28
1:G:642[B]:MET:HA	1:G:642[B]:MET:HE3	1.15	1.13
5:A:806:EDO:O2	6:A:901:HOH:O	1.73	1.05
1:G:642[B]:MET:CA	1:G:642[B]:MET:HE3	1.81	1.04
1:E:536[B]:GLN:HE22	1:E:590[B]:ASN:HD22	1.05	1.03

The worst 5 of 6 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)
6:A:901:HOH:O	6:B:923:HOH:O[2_547]	1.80	0.40
6:C:1437:HOH:O	6:D:1256:HOH:O[2_558]	2.15	0.05
6:A:1105:HOH:O	6:H:3208:HOH:O[2_557]	2.16	0.04
6:C:1345:HOH:O	6:D:1071:HOH:O[2_558]	2.16	0.04
6:E:905:HOH:O	6:H:3813:HOH:O[2_557]	2.19	0.01

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	744/764 (97%)	724 (97%)	19 (3%)	1 (0%)	51	36
1	B	744/764 (97%)	723 (97%)	20 (3%)	1 (0%)	51	36
1	C	756/764 (99%)	735 (97%)	20 (3%)	1 (0%)	51	36
1	D	753/764 (99%)	730 (97%)	22 (3%)	1 (0%)	51	36
1	E	758/764 (99%)	734 (97%)	23 (3%)	1 (0%)	51	36
1	F	736/764 (96%)	716 (97%)	19 (3%)	1 (0%)	51	36
1	G	746/764 (98%)	724 (97%)	18 (2%)	4 (0%)	29	15
1	H	749/764 (98%)	724 (97%)	22 (3%)	3 (0%)	34	21
All	All	5986/6112 (98%)	5810 (97%)	163 (3%)	13 (0%)	47	33

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	569	LEU
1	G	531	GLU
1	H	531	GLU
1	G	746	LYS
1	A	339	VAL

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	632/654 (97%)	626 (99%)	6 (1%)	78	75
1	B	631/654 (96%)	625 (99%)	6 (1%)	76	71
1	C	640/654 (98%)	631 (99%)	9 (1%)	67	59
1	D	642/654 (98%)	631 (98%)	11 (2%)	60	51
1	E	646/654 (99%)	632 (98%)	14 (2%)	52	39
1	F	613/654 (94%)	605 (99%)	8 (1%)	69	62
1	G	636/654 (97%)	626 (98%)	10 (2%)	62	54
1	H	641/654 (98%)	629 (98%)	12 (2%)	57	46
All	All	5081/5232 (97%)	5005 (98%)	76 (2%)	71	56

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	105[A]	SER
1	E	537	TYR
1	H	429[B]	SER
1	E	105[B]	SER
1	E	429[A]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	636	GLN
1	E	358	GLN
1	H	310	HIS
1	D	644	ASN
1	D	764	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 24 are monoatomic - leaving 26 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	EDO	H	804	-	3,3,3	0.23	0	2,2,2	0.78	0
5	EDO	B	804	-	3,3,3	0.34	0	2,2,2	0.25	0
5	EDO	F	805	-	3,3,3	0.59	0	2,2,2	0.40	0
5	EDO	E	805	-	3,3,3	0.33	0	2,2,2	0.64	0
5	EDO	F	804	-	3,3,3	0.42	0	2,2,2	0.25	0
5	EDO	A	806	-	3,3,3	0.50	0	2,2,2	0.32	0
5	EDO	D	807	-	3,3,3	0.49	0	2,2,2	0.70	0
5	EDO	E	804	-	3,3,3	0.32	0	2,2,2	0.30	0
5	EDO	G	805	-	3,3,3	0.34	0	2,2,2	0.09	0
5	EDO	B	805	-	3,3,3	0.69	0	2,2,2	0.47	0
5	EDO	D	805	-	3,3,3	0.36	0	2,2,2	0.15	0
5	EDO	E	806	-	3,3,3	0.50	0	2,2,2	0.66	0
5	EDO	D	804	-	3,3,3	0.47	0	2,2,2	0.58	0
5	EDO	D	808	-	3,3,3	0.61	0	2,2,2	0.38	0
5	EDO	G	807	-	3,3,3	0.19	0	2,2,2	0.11	0
5	EDO	H	805	-	3,3,3	0.18	0	2,2,2	0.59	0
5	EDO	C	805	-	3,3,3	0.51	0	2,2,2	0.10	0
5	EDO	A	805	-	3,3,3	0.76	0	2,2,2	0.42	0
5	EDO	G	806	-	3,3,3	0.54	0	2,2,2	0.46	0
5	EDO	H	806	-	3,3,3	0.65	0	2,2,2	0.27	0
5	EDO	D	806	-	3,3,3	0.23	0	2,2,2	0.59	0
5	EDO	G	804	-	3,3,3	0.37	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	C	806	-	3,3,3	0.63	0	2,2,2	0.16	0
5	EDO	A	804	-	3,3,3	0.49	0	2,2,2	0.46	0
5	EDO	C	804	-	3,3,3	0.25	0	2,2,2	0.82	0
5	EDO	B	806	-	3,3,3	0.42	0	2,2,2	0.56	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	EDO	H	804	-	-	0/1/1/1	-
5	EDO	B	804	-	-	1/1/1/1	-
5	EDO	F	805	-	-	0/1/1/1	-
5	EDO	E	805	-	-	0/1/1/1	-
5	EDO	F	804	-	-	0/1/1/1	-
5	EDO	A	806	-	-	0/1/1/1	-
5	EDO	D	807	-	-	0/1/1/1	-
5	EDO	E	804	-	-	1/1/1/1	-
5	EDO	G	805	-	-	0/1/1/1	-
5	EDO	B	805	-	-	0/1/1/1	-
5	EDO	D	805	-	-	0/1/1/1	-
5	EDO	E	806	-	-	0/1/1/1	-
5	EDO	D	804	-	-	0/1/1/1	-
5	EDO	D	808	-	-	1/1/1/1	-
5	EDO	G	807	-	-	0/1/1/1	-
5	EDO	H	805	-	-	1/1/1/1	-
5	EDO	C	805	-	-	0/1/1/1	-
5	EDO	A	805	-	-	1/1/1/1	-
5	EDO	G	806	-	-	1/1/1/1	-
5	EDO	H	806	-	-	1/1/1/1	-
5	EDO	D	806	-	-	0/1/1/1	-
5	EDO	G	804	-	-	0/1/1/1	-
5	EDO	C	806	-	-	0/1/1/1	-
5	EDO	A	804	-	-	1/1/1/1	-
5	EDO	C	804	-	-	0/1/1/1	-
5	EDO	B	806	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	804	EDO	O1-C1-C2-O2
5	H	805	EDO	O1-C1-C2-O2
5	G	806	EDO	O1-C1-C2-O2
5	E	804	EDO	O1-C1-C2-O2
5	D	808	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	806	EDO	1	0
5	D	808	EDO	2	0
5	G	807	EDO	1	0
5	G	806	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	740/764 (96%)	-0.20	13 (1%) 68 64	16, 27, 49, 97	0
1	B	738/764 (96%)	-0.41	5 (0%) 87 86	14, 23, 39, 70	0
1	C	747/764 (97%)	-0.37	5 (0%) 87 86	14, 22, 38, 87	0
1	D	742/764 (97%)	-0.34	9 (1%) 79 76	14, 23, 38, 82	0
1	E	742/764 (97%)	-0.37	6 (0%) 86 84	15, 22, 37, 104	0
1	F	736/764 (96%)	0.10	22 (2%) 50 44	20, 35, 58, 97	0
1	G	742/764 (97%)	-0.29	6 (0%) 86 84	17, 24, 39, 85	0
1	H	741/764 (96%)	-0.28	5 (0%) 87 86	17, 25, 41, 96	0
All	All	5928/6112 (96%)	-0.27	71 (1%) 79 76	14, 24, 47, 104	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	TYR	8.2
1	E	517	TYR	7.8
1	F	567	VAL	6.0
1	A	569	LEU	5.7
1	C	4	THR	5.2

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 ⓘ

There are no carbohydrates in this entry.

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(Å ²)	Q<0.9
5	EDO	D	805	4/4	0.81	0.22	50,51,54,56	0
3	CA	G	802	1/1	0.83	0.12	38,38,38,38	1
5	EDO	A	805	4/4	0.85	0.12	40,41,43,51	0
3	CA	H	802	1/1	0.85	0.09	39,39,39,39	1
5	EDO	D	807	4/4	0.86	0.11	45,46,48,49	0
5	EDO	E	806	4/4	0.87	0.22	41,42,44,49	0
5	EDO	F	805	4/4	0.87	0.18	45,46,46,49	0
5	EDO	G	805	4/4	0.88	0.18	48,49,56,58	0
5	EDO	F	804	4/4	0.88	0.17	56,57,61,61	0
5	EDO	D	804	4/4	0.88	0.19	44,45,46,53	0
5	EDO	C	805	4/4	0.90	0.11	32,35,36,47	0
5	EDO	E	804	4/4	0.90	0.15	38,44,47,49	0
5	EDO	E	805	4/4	0.90	0.24	25,32,39,52	0
5	EDO	G	807	4/4	0.90	0.19	42,43,46,46	0
5	EDO	B	805	4/4	0.92	0.10	33,34,36,39	0
5	EDO	A	804	4/4	0.92	0.17	34,39,49,53	0
5	EDO	G	804	4/4	0.93	0.10	41,42,44,46	0
5	EDO	H	804	4/4	0.93	0.08	39,43,43,48	0
5	EDO	H	805	4/4	0.93	0.13	42,44,45,50	0
3	CA	E	802	1/1	0.93	0.08	29,29,29,29	1
5	EDO	G	806	4/4	0.93	0.15	37,38,42,45	0
5	EDO	B	806	4/4	0.93	0.08	38,39,40,42	0
4	CL	F	803	1/1	0.94	0.08	36,36,36,36	0
3	CA	F	802	1/1	0.94	0.06	42,42,42,42	1
5	EDO	H	806	4/4	0.94	0.09	30,33,34,35	0
5	EDO	C	806	4/4	0.95	0.11	27,31,33,36	0
4	CL	A	803	1/1	0.95	0.09	34,34,34,34	0
5	EDO	C	804	4/4	0.95	0.13	29,33,33,36	0
2	NA	E	801	1/1	0.95	0.07	24,24,24,24	0
5	EDO	D	806	4/4	0.96	0.09	23,28,35,40	0
5	EDO	D	808	4/4	0.96	0.14	27,30,32,34	0
2	NA	H	801	1/1	0.96	0.07	27,27,27,27	0
3	CA	D	802	1/1	0.96	0.06	30,30,30,30	1
5	EDO	A	806	4/4	0.96	0.12	39,43,43,45	0
2	NA	F	801	1/1	0.97	0.20	34,34,34,34	0
2	NA	D	801	1/1	0.97	0.13	24,24,24,24	0
2	NA	A	801	1/1	0.97	0.09	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	B	804	4/4	0.97	0.17	27,34,40,48	0
3	CA	A	802	1/1	0.97	0.06	38,38,38,38	1
3	CA	C	802	1/1	0.98	0.07	27,27,27,27	1
2	NA	C	801	1/1	0.99	0.06	19,19,19,19	0
2	NA	B	801	1/1	0.99	0.04	21,21,21,21	0
2	NA	G	801	1/1	0.99	0.07	24,24,24,24	0
4	CL	B	803	1/1	0.99	0.07	22,22,22,22	0
3	CA	B	802	1/1	0.99	0.05	31,31,31,31	1
4	CL	D	803	1/1	0.99	0.06	20,20,20,20	0
4	CL	E	803	1/1	1.00	0.08	19,19,19,19	0
4	CL	G	803	1/1	1.00	0.06	21,21,21,21	0
4	CL	C	803	1/1	1.00	0.05	21,21,21,21	0
4	CL	H	803	1/1	1.00	0.06	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.