



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2017 – 06:42 PM EDT

PDB ID : 3FYU
Title : Crystal structure of acetyl xylan esterase from *Bacillus pumilus* obtained in presence of D-xylose and sodium acetate
Authors : Krastanova, I.; Cassetta, A.; Lamba, D.
Deposited on : unknown
Resolution : 2.62 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

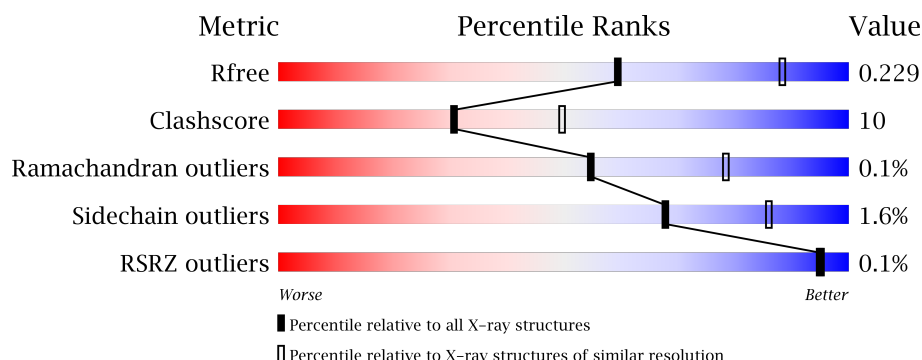
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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}	100719	2983 (2.64-2.60)
Clashscore	112137	3351 (2.64-2.60)
Ramachandran outliers	110173	3298 (2.64-2.60)
Sidechain outliers	110143	3298 (2.64-2.60)
RSRZ outliers	101464	2992 (2.64-2.60)

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. 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	320	
1	I	320	
2	B	320	
2	D	320	
2	H	320	

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Mol	Chain	Length	Quality of chain
3	C	320	 74% 24% ..
3	E	320	 80% 18% ..
3	F	320	 78% 20% ..
3	G	320	 76% 23% ..
3	L	320	 76% 22% ..
3	M	320	 75% 23% ..
3	N	320	 76% 22% ..

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
4	XYP	A	1000	-	-	-	X
4	XYP	C	1001	-	-	-	X
4	XYP	E	1002	-	-	-	X
4	XYP	I	1004	-	-	-	X
4	XYP	L	1005	-	-	-	X
4	XYP	M	1003	-	-	-	X
4	XYP	N	1006	-	-	-	X
5	EDO	A	321	-	-	-	X
5	EDO	B	321	-	-	-	X
5	EDO	D	321	-	-	-	X
5	EDO	G	322	-	-	-	X
5	EDO	I	322	-	-	-	X
5	EDO	N	321	-	-	-	X
6	CL	N	322	-	-	X	-
7	ACY	C	321	-	-	-	X
7	ACY	E	321	-	-	-	X
7	ACY	F	321	-	-	-	X
7	ACY	G	321	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 31382 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 Acetyl xylan esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2547	1654	417	472	4			
1	I	316	Total	C	N	O	S	0	0	0
			2531	1643	415	470	3			

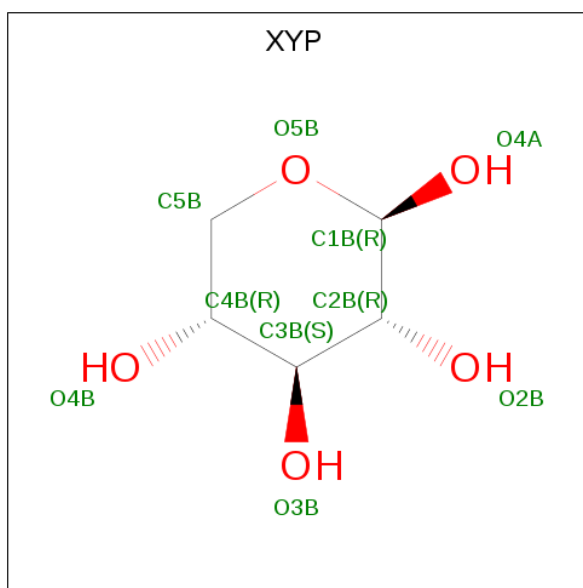
- Molecule 2 is a protein called Acetyl xylan esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	318	Total	C	N	O	S	0	0	0
			2548	1654	417	473	4			
2	D	317	Total	C	N	O	S	0	0	0
			2540	1648	416	472	4			
2	H	316	Total	C	N	O	S	0	0	0
			2532	1643	415	471	3			

- Molecule 3 is a protein called Acetyl xylan esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	316	Total	C	N	O	S	0	0	0
			2528	1641	415	469	3			
3	E	317	Total	C	N	O	S	0	0	0
			2536	1646	416	470	4			
3	F	316	Total	C	N	O	S	0	0	0
			2528	1641	415	469	3			
3	G	316	Total	C	N	O	S	0	0	0
			2528	1641	415	469	3			
3	L	317	Total	C	N	O	S	0	0	0
			2536	1646	416	470	4			
3	M	317	Total	C	N	O	S	0	0	0
			2536	1646	416	470	4			
3	N	316	Total	C	N	O	S	0	0	0
			2528	1641	415	469	3			

- Molecule 4 is BETA-D-XYLOPYRANOSE (three-letter code: XYP) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		
4	C	1	Total	C	O	0	0
			10	5	5		
4	E	1	Total	C	O	0	0
			10	5	5		
4	I	1	Total	C	O	0	0
			10	5	5		
4	L	1	Total	C	O	0	0
			10	5	5		
4	M	1	Total	C	O	0	0
			10	5	5		
4	N	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

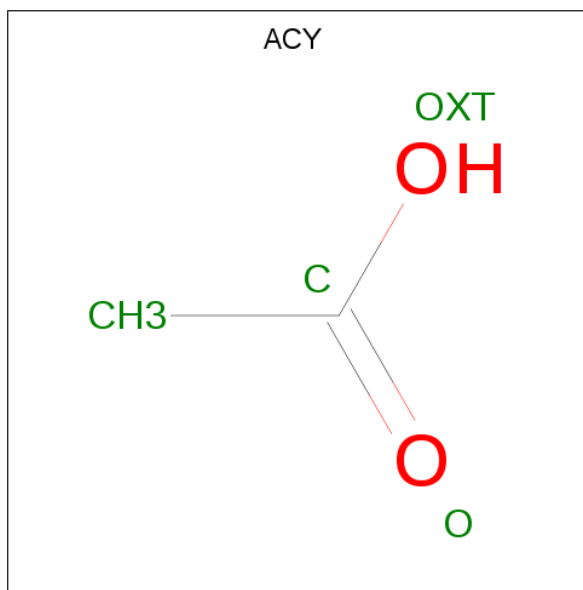


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	N	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	2	Total Cl 2 2	0	0
6	D	1	Total Cl 1 1	0	0
6	E	2	Total Cl 2 2	0	0
6	H	2	Total Cl 2 2	0	0
6	B	1	Total Cl 1 1	0	0
6	I	1	Total Cl 1 1	0	0
6	C	2	Total Cl 2 2	0	0
6	A	2	Total Cl 2 2	0	0
6	N	2	Total Cl 2 2	0	0
6	L	1	Total Cl 1 1	0	0
6	F	1	Total Cl 1 1	0	0
6	M	1	Total Cl 1 1	0	0

- Molecule 7 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

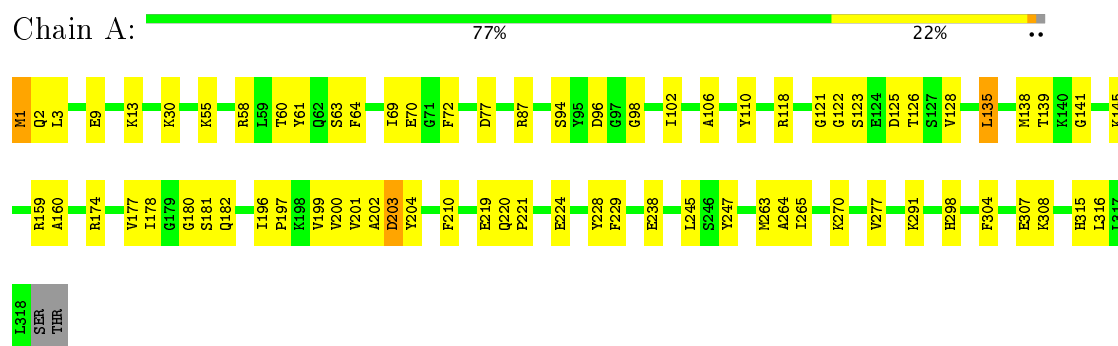
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	91	Total O 91 91	0	0
8	B	66	Total O 66 66	0	0
8	C	78	Total O 78 78	0	0
8	D	68	Total O 68 68	0	0
8	E	77	Total O 77 77	0	0
8	F	72	Total O 72 72	0	0
8	G	51	Total O 51 51	0	0
8	H	69	Total O 69 69	0	0
8	I	68	Total O 68 68	0	0
8	L	68	Total O 68 68	0	0
8	M	52	Total O 52 52	0	0
8	N	44	Total O 44 44	0	0

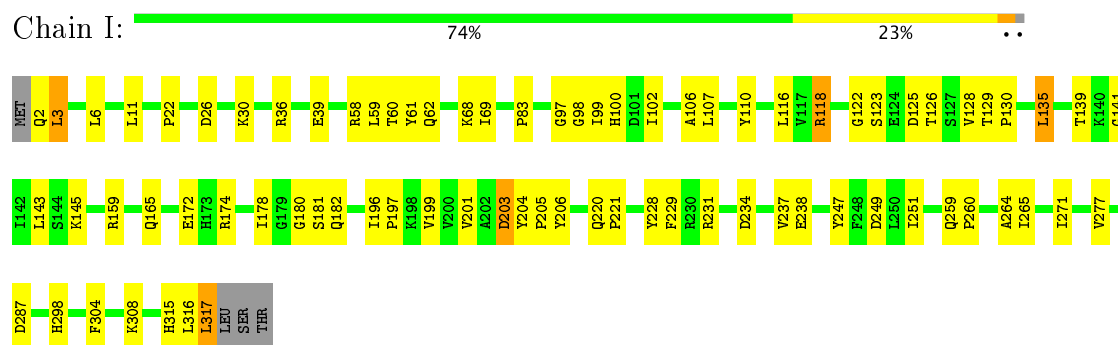
3 Residue-property plots [i](#)

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.

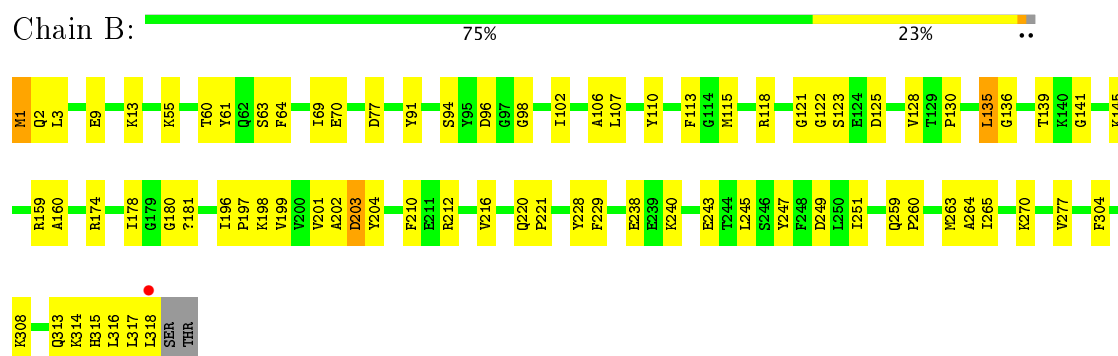
- Molecule 1: Acetyl xylan esterase



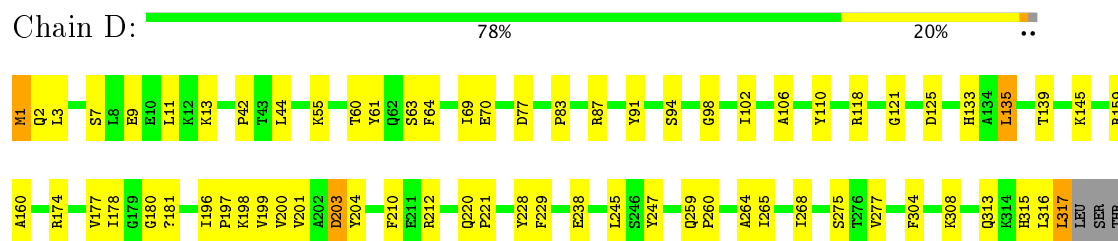
- Molecule 1: Acetyl xylan esterase



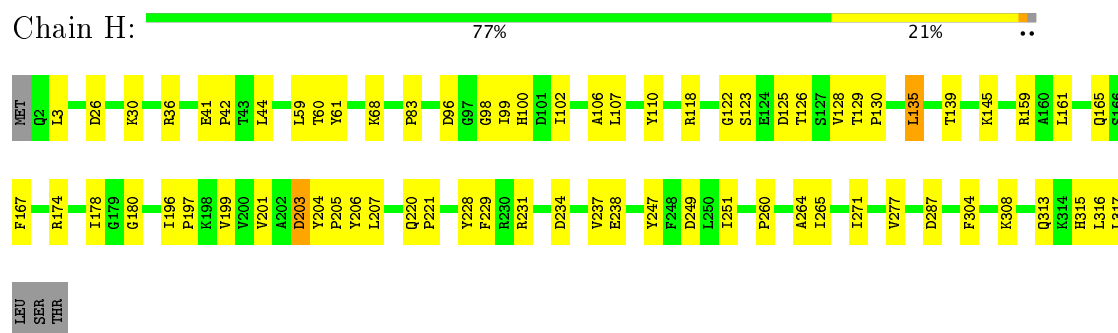
- Molecule 2: Acetyl xylan esterase



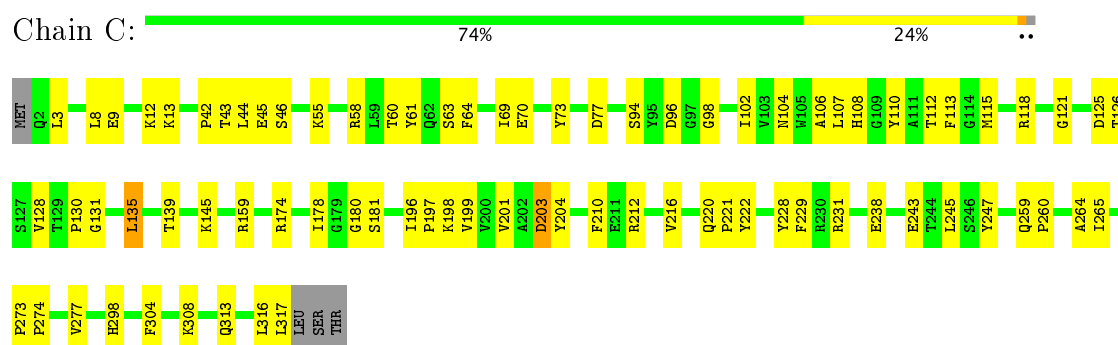
- Molecule 2: Acetyl xylan esterase



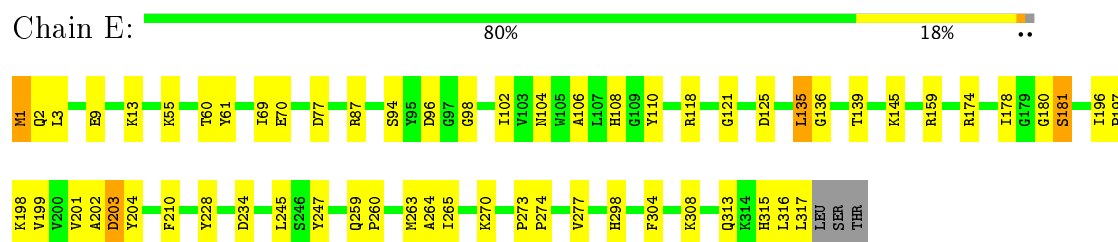
- Molecule 2: Acetyl xylan esterase



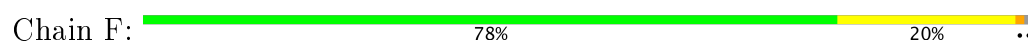
- Molecule 3: Acetyl xylan esterase

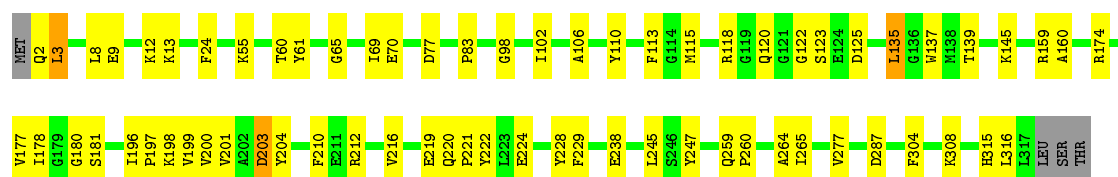


- Molecule 3: Acetyl xylan esterase



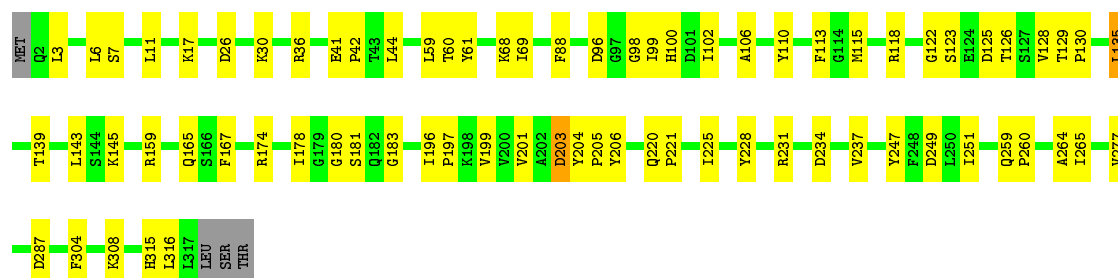
- Molecule 3: Acetyl xylan esterase





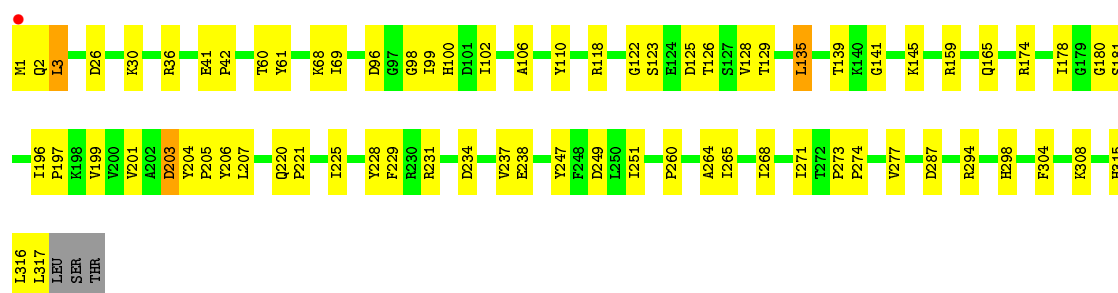
- Molecule 3: Acetyl xylan esterase

Chain G: 76% 23% ..



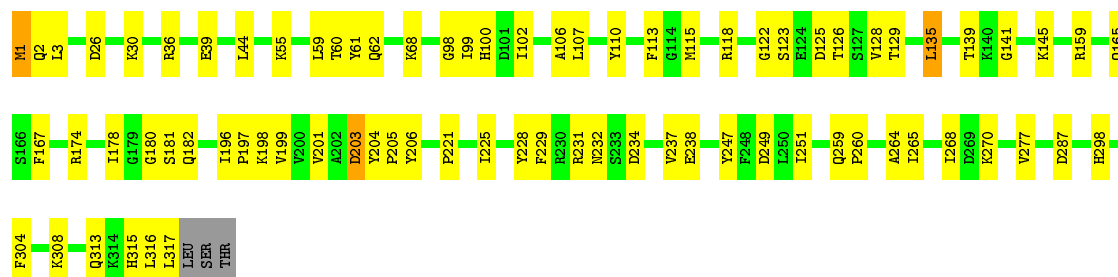
- Molecule 3: Acetyl xylan esterase

Chain L: 76% 22% ..



- Molecule 3: Acetyl xylan esterase

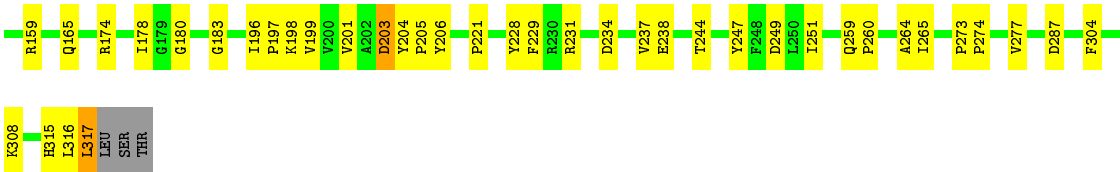
Chain M: 75% 23% ..



- Molecule 3: Acetyl xylan esterase

Chain N: 76% 22% ..





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	142.22Å 86.62Å 183.97Å 90.00° 112.78° 90.00°	Depositor
Resolution (Å)	26.88 – 2.62 26.88 – 2.62	Depositor EDS
% Data completeness (in resolution range)	86.0 (26.88-2.62) 86.0 (26.88-2.62)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.230 0.196 , 0.229	Depositor DCC
R_{free} test set	10592 reflections (9.91%)	DCC
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.688	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , -2.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.129 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31382	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: XYP, CL, EDO, TIS, OAS, ACY

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	0/2609	0.60	0/3540
1	I	0.38	0/2593	0.58	0/3519
2	B	0.39	0/2609	0.60	0/3540
2	D	0.39	0/2601	0.59	0/3529
2	H	0.38	0/2593	0.58	0/3519
3	C	0.38	0/2600	0.60	0/3530
3	E	0.39	0/2608	0.60	0/3540
3	F	0.39	0/2600	0.60	0/3530
3	G	0.38	0/2600	0.58	0/3530
3	L	0.37	0/2608	0.59	0/3540
3	M	0.38	0/2608	0.58	0/3540
3	N	0.38	0/2600	0.58	0/3530
All	All	0.38	0/31229	0.59	0/42387

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	2547	0	2495	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2531	0	2472	65	0
2	B	2548	0	2497	55	0
2	D	2540	0	2486	51	0
2	H	2532	0	2474	55	0
3	C	2528	0	2471	59	0
3	E	2536	0	2483	44	0
3	F	2528	0	2471	47	0
3	G	2528	0	2471	56	0
3	L	2536	0	2483	54	0
3	M	2536	0	2483	65	0
3	N	2528	0	2471	60	0
4	A	10	0	10	1	0
4	C	10	0	10	1	0
4	E	10	0	10	1	0
4	I	10	0	10	1	0
4	L	10	0	10	1	0
4	M	10	0	10	2	0
4	N	10	0	10	2	0
5	A	4	0	6	0	0
5	B	8	0	12	1	0
5	D	8	0	12	0	0
5	E	4	0	6	0	0
5	F	8	0	12	1	0
5	G	4	0	6	0	0
5	H	4	0	6	2	0
5	I	4	0	6	0	0
5	M	4	0	6	0	0
5	N	4	0	6	0	0
6	A	2	0	0	1	0
6	B	1	0	0	1	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	1	0
6	I	1	0	0	1	0
6	L	1	0	0	1	0
6	M	1	0	0	1	0
6	N	2	0	0	2	0
7	C	4	0	3	0	0
7	E	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	4	0	3	0	0
7	G	4	0	3	0	0
7	I	4	0	3	0	0
8	A	91	0	0	4	0
8	B	66	0	0	1	0
8	C	78	0	0	3	0
8	D	68	0	0	1	0
8	E	77	0	0	1	0
8	F	72	0	0	6	0
8	G	51	0	0	2	0
8	H	69	0	0	1	0
8	I	68	0	0	2	0
8	L	68	0	0	0	0
8	M	52	0	0	3	0
8	N	44	0	0	2	0
All	All	31382	0	29920	629	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 10.

The worst 5 of 629 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)
3:M:1:MET:HE2	3:M:2:GLN:H	1.32	0.94
3:E:1:MET:SD	3:E:2:GLN:N	2.42	0.93
3:C:313:GLN:HG3	3:C:317:LEU:HD12	1.59	0.82
2:H:206:TYR:OH	2:H:221:PRO:HG2	1.82	0.80
1:I:206:TYR:OH	1:I:221:PRO:HG2	1.83	0.78

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	315/320 (98%)	300 (95%)	15 (5%)	0	100	100
1	I	313/320 (98%)	294 (94%)	18 (6%)	1 (0%)	44	68
2	B	315/320 (98%)	300 (95%)	15 (5%)	0	100	100
2	D	314/320 (98%)	301 (96%)	13 (4%)	0	100	100
2	H	313/320 (98%)	293 (94%)	20 (6%)	0	100	100
3	C	314/320 (98%)	300 (96%)	14 (4%)	0	100	100
3	E	315/320 (98%)	300 (95%)	14 (4%)	1 (0%)	44	68
3	F	314/320 (98%)	299 (95%)	15 (5%)	0	100	100
3	G	314/320 (98%)	293 (93%)	21 (7%)	0	100	100
3	L	315/320 (98%)	295 (94%)	20 (6%)	0	100	100
3	M	315/320 (98%)	295 (94%)	20 (6%)	0	100	100
3	N	314/320 (98%)	292 (93%)	22 (7%)	0	100	100
All	All	3771/3840 (98%)	3562 (94%)	207 (6%)	2 (0%)	55	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	181	SER
1	I	118	ARG

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/269 (99%)	263 (98%)	4 (2%)	70	87
1	I	265/269 (98%)	260 (98%)	5 (2%)	62	83
2	B	267/269 (99%)	263 (98%)	4 (2%)	70	87
2	D	266/269 (99%)	261 (98%)	5 (2%)	62	83
2	H	265/269 (98%)	261 (98%)	4 (2%)	70	87
3	C	266/270 (98%)	263 (99%)	3 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	267/270 (99%)	263 (98%)	4 (2%)	70	87
3	F	266/270 (98%)	263 (99%)	3 (1%)	78	91
3	G	266/270 (98%)	262 (98%)	4 (2%)	70	87
3	L	267/270 (99%)	263 (98%)	4 (2%)	70	87
3	M	267/270 (99%)	262 (98%)	5 (2%)	62	83
3	N	266/270 (98%)	261 (98%)	5 (2%)	62	83
All	All	3195/3235 (99%)	3145 (98%)	50 (2%)	68	86

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	203	ASP
2	H	3	LEU
3	N	135	LEU
3	G	3	LEU
3	G	165	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	62	GLN
3	G	298	HIS
3	L	62	GLN
3	G	37	GLN
3	L	37	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	OAS	A	181	1	8,8,9	1.58	2 (25%)	6,9,11	3.48	2 (33%)
2	TIS	B	181	2	6,9,10	1.50	1 (16%)	4,12,14	1.02	0
2	TIS	D	181	2	6,9,10	1.20	1 (16%)	4,12,14	1.10	0
2	TIS	H	181	2	6,9,10	1.59	1 (16%)	4,12,14	1.01	0
1	OAS	I	181	1	8,8,9	1.52	3 (37%)	6,9,11	2.58	2 (33%)

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
1	OAS	A	181	1	-	0/5/7/9	0/0/0/0
2	TIS	B	181	2	-	0/3/8/10	0/0/0/0
2	TIS	D	181	2	-	0/3/8/10	0/0/0/0
2	TIS	H	181	2	-	0/3/8/10	0/0/0/0
1	OAS	I	181	1	-	0/5/7/9	0/0/0/0

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	181	OAS	OG-C1A	-2.08	1.23	1.33
2	D	181	TIS	C2T-C1T	2.14	1.53	1.50
1	I	181	OAS	CA-C	2.15	1.53	1.50
1	A	181	OAS	CA-C	2.19	1.53	1.50
1	I	181	OAS	OAC-C1A	2.61	1.30	1.20

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	OAS	OG-C1A-C2A	2.55	123.93	112.44
1	I	181	OAS	OG-C1A-C2A	2.56	123.95	112.44
1	I	181	OAS	CB-OG-C1A	5.10	130.15	117.17
1	A	181	OAS	CB-OG-C1A	7.52	136.30	117.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	181	OAS	2	0
2	B	181	TIS	1	0
2	D	181	TIS	1	0
1	I	181	OAS	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 18 are monoatomic - leaving 25 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	$\# Z > 2$
4	XYP	A	1000	-	10,10,10	1.05	0	14,14,14	0.97	0
5	EDO	A	321	-	3,3,3	0.59	0	2,2,2	0.27	0
5	EDO	B	321	-	3,3,3	0.47	0	2,2,2	0.42	0
5	EDO	B	322	-	3,3,3	0.61	0	2,2,2	0.28	0
4	XYP	C	1001	-	10,10,10	1.15	0	14,14,14	0.97	0
7	ACY	C	321	-	1,3,3	3.05	1 (100%)	0,3,3	0.00	-
5	EDO	D	321	-	3,3,3	0.60	0	2,2,2	0.21	0
5	EDO	D	322	-	3,3,3	0.55	0	2,2,2	0.27	0
4	XYP	E	1002	-	10,10,10	1.05	0	14,14,14	0.99	0
7	ACY	E	321	-	1,3,3	1.99	0	0,3,3	0.00	-
5	EDO	E	322	-	3,3,3	0.51	0	2,2,2	0.36	0
7	ACY	F	321	-	1,3,3	2.57	1 (100%)	0,3,3	0.00	-
5	EDO	F	322	-	3,3,3	0.49	0	2,2,2	0.29	0
5	EDO	F	323	-	3,3,3	0.59	0	2,2,2	0.30	0
7	ACY	G	321	-	1,3,3	3.14	1 (100%)	0,3,3	0.00	-
5	EDO	G	322	-	3,3,3	0.57	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	H	321	-	3,3,3	0.59	0	2,2,2	0.23	0
4	XYP	I	1004	-	10,10,10	1.19	1 (10%)	14,14,14	0.97	0
7	ACY	I	321	-	1,3,3	3.01	1 (100%)	0,3,3	0.00	-
5	EDO	I	322	-	3,3,3	0.49	0	2,2,2	0.35	0
4	XYP	L	1005	-	10,10,10	1.21	1 (10%)	14,14,14	0.99	0
4	XYP	M	1003	-	10,10,10	1.11	0	14,14,14	0.91	0
5	EDO	M	321	-	3,3,3	0.64	0	2,2,2	0.22	0
4	XYP	N	1006	-	10,10,10	1.12	0	14,14,14	0.92	0
5	EDO	N	321	-	3,3,3	0.61	0	2,2,2	0.27	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
4	XYP	A	1000	-	-	0/0/17/17	0/1/1/1
5	EDO	A	321	-	-	0/1/1/1	0/0/0/0
5	EDO	B	321	-	-	0/1/1/1	0/0/0/0
5	EDO	B	322	-	-	0/1/1/1	0/0/0/0
4	XYP	C	1001	-	-	0/0/17/17	0/1/1/1
7	ACY	C	321	-	-	0/0/0/0	0/0/0/0
5	EDO	D	321	-	-	0/1/1/1	0/0/0/0
5	EDO	D	322	-	-	0/1/1/1	0/0/0/0
4	XYP	E	1002	-	-	0/0/17/17	0/1/1/1
7	ACY	E	321	-	-	0/0/0/0	0/0/0/0
5	EDO	E	322	-	-	0/1/1/1	0/0/0/0
7	ACY	F	321	-	-	0/0/0/0	0/0/0/0
5	EDO	F	322	-	-	0/1/1/1	0/0/0/0
5	EDO	F	323	-	-	0/1/1/1	0/0/0/0
7	ACY	G	321	-	-	0/0/0/0	0/0/0/0
5	EDO	G	322	-	-	0/1/1/1	0/0/0/0
5	EDO	H	321	-	-	0/1/1/1	0/0/0/0
4	XYP	I	1004	-	-	0/0/17/17	0/1/1/1
7	ACY	I	321	-	-	0/0/0/0	0/0/0/0
5	EDO	I	322	-	-	0/1/1/1	0/0/0/0
4	XYP	L	1005	-	-	0/0/17/17	0/1/1/1
4	XYP	M	1003	-	-	0/0/17/17	0/1/1/1
5	EDO	M	321	-	-	0/1/1/1	0/0/0/0
4	XYP	N	1006	-	-	0/0/17/17	0/1/1/1
5	EDO	N	321	-	-	0/1/1/1	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1005	XYP	O5B-C1B	-2.27	1.39	1.43
4	I	1004	XYP	O5B-C1B	-2.17	1.40	1.43
7	F	321	ACY	CH3-C	2.57	1.52	1.48
7	I	321	ACY	CH3-C	3.01	1.52	1.48
7	C	321	ACY	CH3-C	3.05	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1000	XYP	1	0
5	B	322	EDO	1	0
4	C	1001	XYP	1	0
4	E	1002	XYP	1	0
5	F	323	EDO	1	0
5	H	321	EDO	2	0
4	I	1004	XYP	1	0
4	L	1005	XYP	1	0
4	M	1003	XYP	2	0
4	N	1006	XYP	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	317/320 (99%)	-0.65	0 100 100	7, 15, 26, 41	0
1	I	315/320 (98%)	-0.57	0 100 100	11, 19, 31, 38	0
2	B	317/320 (99%)	-0.63	1 (0%) 93 93	7, 15, 28, 39	0
2	D	316/320 (98%)	-0.63	0 100 100	8, 17, 28, 36	0
2	H	315/320 (98%)	-0.57	0 100 100	9, 21, 31, 37	0
3	C	316/320 (98%)	-0.65	0 100 100	7, 16, 27, 32	0
3	E	317/320 (99%)	-0.62	0 100 100	7, 16, 26, 33	0
3	F	316/320 (98%)	-0.62	0 100 100	9, 17, 29, 35	0
3	G	316/320 (98%)	-0.54	0 100 100	12, 20, 32, 39	0
3	L	317/320 (99%)	-0.55	1 (0%) 93 93	12, 20, 30, 44	0
3	M	317/320 (99%)	-0.53	0 100 100	12, 22, 33, 41	0
3	N	316/320 (98%)	-0.53	0 100 100	10, 21, 31, 39	0
All	All	3795/3840 (98%)	-0.59	2 (0%) 95 95	7, 19, 30, 44	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	318	LEU	2.8
3	L	1	MET	2.1

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	TIS	H	181	10/11	0.91	0.18	-	22,25,32,32	0
1	OAS	A	181	9/10	0.92	0.16	-	17,18,31,31	0
2	TIS	B	181	10/11	0.93	0.15	-	13,15,22,22	0
2	TIS	D	181	10/11	0.94	0.12	-	16,19,23,24	0
1	OAS	I	181	9/10	0.94	0.16	-	18,21,30,30	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
7	ACY	F	321	4/4	0.95	0.22	8.07	29,30,30,30	0
5	EDO	A	321	4/4	0.88	0.19	7.12	18,22,23,24	0
5	EDO	D	321	4/4	0.86	0.16	5.46	25,26,26,26	0
4	XYP	I	1004	10/10	0.86	0.26	5.33	34,36,38,39	0
5	EDO	G	322	4/4	0.84	0.20	4.70	23,25,26,27	0
4	XYP	L	1005	10/10	0.88	0.24	4.43	37,38,39,41	0
7	ACY	E	321	4/4	0.94	0.20	4.40	25,27,27,29	0
5	EDO	B	321	4/4	0.88	0.21	4.34	36,36,36,37	0
4	XYP	N	1006	10/10	0.88	0.24	4.08	33,37,39,40	0
5	EDO	I	322	4/4	0.93	0.17	3.96	28,30,32,33	0
4	XYP	C	1001	10/10	0.88	0.20	3.61	33,35,38,38	0
4	XYP	A	1000	10/10	0.90	0.24	3.50	36,38,39,39	0
4	XYP	E	1002	10/10	0.91	0.20	3.44	35,36,37,38	0
7	ACY	G	321	4/4	0.92	0.20	3.03	38,39,40,40	0
7	ACY	C	321	4/4	0.91	0.15	2.36	24,24,26,26	0
4	XYP	M	1003	10/10	0.91	0.18	2.31	39,40,41,41	0
5	EDO	N	321	4/4	0.89	0.18	2.02	26,27,28,29	0
5	EDO	F	322	4/4	0.91	0.17	1.98	19,21,22,22	0
5	EDO	B	322	4/4	0.89	0.17	1.57	23,23,24,25	0
6	CL	G	323	1/1	0.96	0.13	1.06	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	EDO	M	321	4/4	0.87	0.15	0.77	32,32,33,33	0
7	ACY	I	321	4/4	0.90	0.13	-0.01	38,39,39,39	0
6	CL	E	324	1/1	0.97	0.12	-0.47	40,40,40,40	0
5	EDO	H	321	4/4	0.93	0.14	-0.54	24,25,26,27	0
6	CL	G	324	1/1	0.95	0.12	-0.56	37,37,37,37	0
6	CL	A	323	1/1	0.95	0.09	-0.88	31,31,31,31	0
5	EDO	E	322	4/4	0.93	0.10	-1.17	23,24,24,25	0
6	CL	C	323	1/1	0.97	0.08	-1.34	41,41,41,41	0
6	CL	M	322	1/1	0.99	0.11	-1.35	33,33,33,33	0
6	CL	N	323	1/1	0.93	0.08	-1.53	44,44,44,44	0
6	CL	E	323	1/1	1.00	0.10	-1.62	20,20,20,20	0
6	CL	D	323	1/1	0.98	0.07	-1.78	21,21,21,21	0
6	CL	F	324	1/1	0.98	0.09	-2.16	25,25,25,25	0
6	CL	N	322	1/1	0.99	0.07	-2.31	25,25,25,25	0
6	CL	H	323	1/1	0.98	0.05	-2.83	38,38,38,38	0
6	CL	A	322	1/1	0.99	0.08	-2.94	17,17,17,17	0
6	CL	H	322	1/1	0.97	0.07	-3.34	20,20,20,20	0
6	CL	L	321	1/1	0.99	0.06	-3.34	27,27,27,27	0
6	CL	C	322	1/1	0.99	0.07	-3.81	20,20,20,20	0
6	CL	I	323	1/1	0.99	0.06	-4.38	18,18,18,18	0
6	CL	B	323	1/1	0.98	0.04	-4.66	22,22,22,22	0
5	EDO	D	322	4/4	0.89	0.17	-	25,28,28,28	0
5	EDO	F	323	4/4	0.88	0.18	-	31,32,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.