Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2023 – 12:36 AM EDT

PDB ID	:	3UG5
Title	:	Crystal structure of alpha-L-arabinofuranosidase from Thermotoga maritima xylose complex
Authors	:	Im, D.-H.; Miyazaki, K.; Wakagi, T.; Fushinobu, S.
Deposited on	:	2011-11-02
Resolution	:	2.30 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:

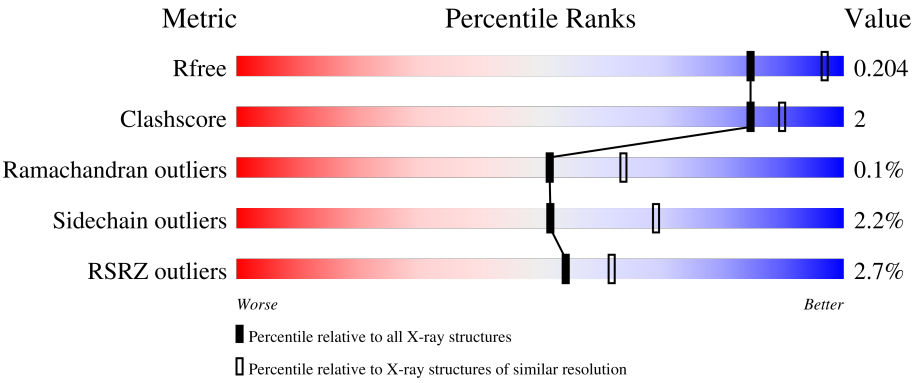
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	504	2% 88% 7% ·
1	B	504	4% 87% 7% · ·
1	C	504	3% 89% 7% ·
1	D	504	3% 85% 9% · 5%
1	E	504	2% 88% 7% · ·

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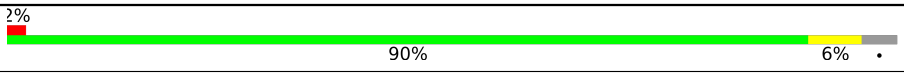
Mol	Chain	Length	Quality of chain
1	F	504	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 24750 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 Alpha-L-arabinofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3876	2488	644	729	15			
1	B	482	Total	C	N	O	S	0	0	0
			3876	2488	644	729	15			
1	C	483	Total	C	N	O	S	0	0	0
			3885	2493	645	732	15			
1	D	481	Total	C	N	O	S	0	0	0
			3868	2482	643	728	15			
1	E	482	Total	C	N	O	S	0	0	0
			3876	2488	644	729	15			
1	F	482	Total	C	N	O	S	0	0	0
			3876	2488	644	729	15			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q9WYB7
A	-18	GLY	-	expression tag	UNP Q9WYB7
A	-17	SER	-	expression tag	UNP Q9WYB7
A	-16	SER	-	expression tag	UNP Q9WYB7
A	-15	HIS	-	expression tag	UNP Q9WYB7
A	-14	HIS	-	expression tag	UNP Q9WYB7
A	-13	HIS	-	expression tag	UNP Q9WYB7
A	-12	HIS	-	expression tag	UNP Q9WYB7
A	-11	HIS	-	expression tag	UNP Q9WYB7
A	-10	HIS	-	expression tag	UNP Q9WYB7
A	-9	SER	-	expression tag	UNP Q9WYB7
A	-8	SER	-	expression tag	UNP Q9WYB7
A	-7	GLY	-	expression tag	UNP Q9WYB7
A	-6	LEU	-	expression tag	UNP Q9WYB7
A	-5	VAL	-	expression tag	UNP Q9WYB7
A	-4	PRO	-	expression tag	UNP Q9WYB7
A	-3	ARG	-	expression tag	UNP Q9WYB7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9WYB7
A	-1	SER	-	expression tag	UNP Q9WYB7
A	0	HIS	-	expression tag	UNP Q9WYB7
A	4	GLY	ARG	engineered mutation	UNP Q9WYB7
B	-19	MET	-	expression tag	UNP Q9WYB7
B	-18	GLY	-	expression tag	UNP Q9WYB7
B	-17	SER	-	expression tag	UNP Q9WYB7
B	-16	SER	-	expression tag	UNP Q9WYB7
B	-15	HIS	-	expression tag	UNP Q9WYB7
B	-14	HIS	-	expression tag	UNP Q9WYB7
B	-13	HIS	-	expression tag	UNP Q9WYB7
B	-12	HIS	-	expression tag	UNP Q9WYB7
B	-11	HIS	-	expression tag	UNP Q9WYB7
B	-10	HIS	-	expression tag	UNP Q9WYB7
B	-9	SER	-	expression tag	UNP Q9WYB7
B	-8	SER	-	expression tag	UNP Q9WYB7
B	-7	GLY	-	expression tag	UNP Q9WYB7
B	-6	LEU	-	expression tag	UNP Q9WYB7
B	-5	VAL	-	expression tag	UNP Q9WYB7
B	-4	PRO	-	expression tag	UNP Q9WYB7
B	-3	ARG	-	expression tag	UNP Q9WYB7
B	-2	GLY	-	expression tag	UNP Q9WYB7
B	-1	SER	-	expression tag	UNP Q9WYB7
B	0	HIS	-	expression tag	UNP Q9WYB7
B	4	GLY	ARG	engineered mutation	UNP Q9WYB7
C	-19	MET	-	expression tag	UNP Q9WYB7
C	-18	GLY	-	expression tag	UNP Q9WYB7
C	-17	SER	-	expression tag	UNP Q9WYB7
C	-16	SER	-	expression tag	UNP Q9WYB7
C	-15	HIS	-	expression tag	UNP Q9WYB7
C	-14	HIS	-	expression tag	UNP Q9WYB7
C	-13	HIS	-	expression tag	UNP Q9WYB7
C	-12	HIS	-	expression tag	UNP Q9WYB7
C	-11	HIS	-	expression tag	UNP Q9WYB7
C	-10	HIS	-	expression tag	UNP Q9WYB7
C	-9	SER	-	expression tag	UNP Q9WYB7
C	-8	SER	-	expression tag	UNP Q9WYB7
C	-7	GLY	-	expression tag	UNP Q9WYB7
C	-6	LEU	-	expression tag	UNP Q9WYB7
C	-5	VAL	-	expression tag	UNP Q9WYB7
C	-4	PRO	-	expression tag	UNP Q9WYB7
C	-3	ARG	-	expression tag	UNP Q9WYB7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q9WYB7
C	-1	SER	-	expression tag	UNP Q9WYB7
C	0	HIS	-	expression tag	UNP Q9WYB7
C	4	GLY	ARG	engineered mutation	UNP Q9WYB7
D	-19	MET	-	expression tag	UNP Q9WYB7
D	-18	GLY	-	expression tag	UNP Q9WYB7
D	-17	SER	-	expression tag	UNP Q9WYB7
D	-16	SER	-	expression tag	UNP Q9WYB7
D	-15	HIS	-	expression tag	UNP Q9WYB7
D	-14	HIS	-	expression tag	UNP Q9WYB7
D	-13	HIS	-	expression tag	UNP Q9WYB7
D	-12	HIS	-	expression tag	UNP Q9WYB7
D	-11	HIS	-	expression tag	UNP Q9WYB7
D	-10	HIS	-	expression tag	UNP Q9WYB7
D	-9	SER	-	expression tag	UNP Q9WYB7
D	-8	SER	-	expression tag	UNP Q9WYB7
D	-7	GLY	-	expression tag	UNP Q9WYB7
D	-6	LEU	-	expression tag	UNP Q9WYB7
D	-5	VAL	-	expression tag	UNP Q9WYB7
D	-4	PRO	-	expression tag	UNP Q9WYB7
D	-3	ARG	-	expression tag	UNP Q9WYB7
D	-2	GLY	-	expression tag	UNP Q9WYB7
D	-1	SER	-	expression tag	UNP Q9WYB7
D	0	HIS	-	expression tag	UNP Q9WYB7
D	4	GLY	ARG	engineered mutation	UNP Q9WYB7
E	-19	MET	-	expression tag	UNP Q9WYB7
E	-18	GLY	-	expression tag	UNP Q9WYB7
E	-17	SER	-	expression tag	UNP Q9WYB7
E	-16	SER	-	expression tag	UNP Q9WYB7
E	-15	HIS	-	expression tag	UNP Q9WYB7
E	-14	HIS	-	expression tag	UNP Q9WYB7
E	-13	HIS	-	expression tag	UNP Q9WYB7
E	-12	HIS	-	expression tag	UNP Q9WYB7
E	-11	HIS	-	expression tag	UNP Q9WYB7
E	-10	HIS	-	expression tag	UNP Q9WYB7
E	-9	SER	-	expression tag	UNP Q9WYB7
E	-8	SER	-	expression tag	UNP Q9WYB7
E	-7	GLY	-	expression tag	UNP Q9WYB7
E	-6	LEU	-	expression tag	UNP Q9WYB7
E	-5	VAL	-	expression tag	UNP Q9WYB7
E	-4	PRO	-	expression tag	UNP Q9WYB7
E	-3	ARG	-	expression tag	UNP Q9WYB7

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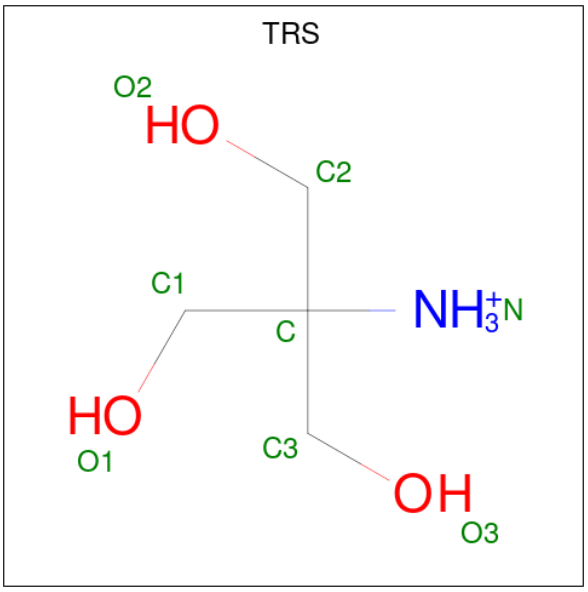
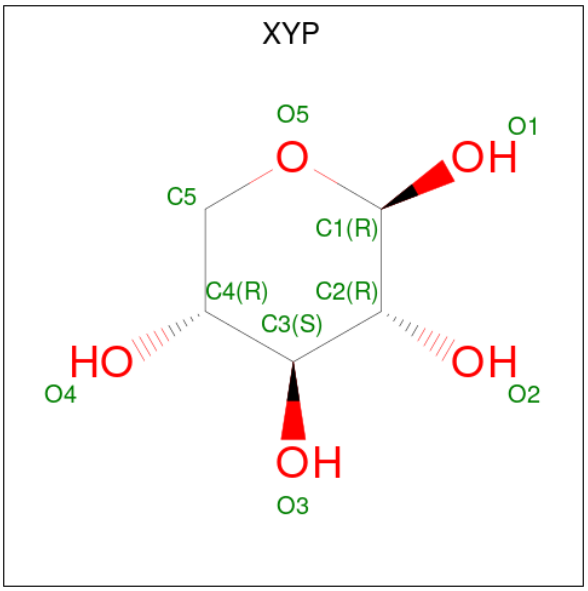
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q9WYB7
E	-1	SER	-	expression tag	UNP Q9WYB7
E	0	HIS	-	expression tag	UNP Q9WYB7
E	4	GLY	ARG	engineered mutation	UNP Q9WYB7
F	-19	MET	-	expression tag	UNP Q9WYB7
F	-18	GLY	-	expression tag	UNP Q9WYB7
F	-17	SER	-	expression tag	UNP Q9WYB7
F	-16	SER	-	expression tag	UNP Q9WYB7
F	-15	HIS	-	expression tag	UNP Q9WYB7
F	-14	HIS	-	expression tag	UNP Q9WYB7
F	-13	HIS	-	expression tag	UNP Q9WYB7
F	-12	HIS	-	expression tag	UNP Q9WYB7
F	-11	HIS	-	expression tag	UNP Q9WYB7
F	-10	HIS	-	expression tag	UNP Q9WYB7
F	-9	SER	-	expression tag	UNP Q9WYB7
F	-8	SER	-	expression tag	UNP Q9WYB7
F	-7	GLY	-	expression tag	UNP Q9WYB7
F	-6	LEU	-	expression tag	UNP Q9WYB7
F	-5	VAL	-	expression tag	UNP Q9WYB7
F	-4	PRO	-	expression tag	UNP Q9WYB7
F	-3	ARG	-	expression tag	UNP Q9WYB7
F	-2	GLY	-	expression tag	UNP Q9WYB7
F	-1	SER	-	expression tag	UNP Q9WYB7
F	0	HIS	-	expression tag	UNP Q9WYB7
F	4	GLY	ARG	engineered mutation	UNP Q9WYB7

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		
2	C	1	Total	C	N	O	0	0
			8	4	1	3		
2	C	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		
2	E	1	Total	C	N	O	0	0
			8	4	1	3		
2	E	1	Total	C	N	O	0	0
			8	4	1	3		
2	F	1	Total	C	N	O	0	0
			8	4	1	3		
2	F	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is beta-D-xylopyranose (three-letter code: XYP) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 5 5	0	0
3	A	1	Total C O 10 5 5	0	0
3	A	1	Total C O 10 5 5	0	0
3	B	1	Total C O 10 5 5	0	0
3	B	1	Total C O 10 5 5	0	0
3	B	1	Total C O 10 5 5	0	0
3	C	1	Total C O 10 5 5	0	0
3	C	1	Total C O 10 5 5	0	0
3	D	1	Total C O 10 5 5	0	0
3	D	1	Total C O 10 5 5	0	0
3	D	1	Total C O 10 5 5	0	0
3	D	1	Total C O 10 5 5	0	0
3	E	1	Total C O 10 5 5	0	0
3	E	1	Total C O 10 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 10 5 5	0	0

- Molecule 4 is water.

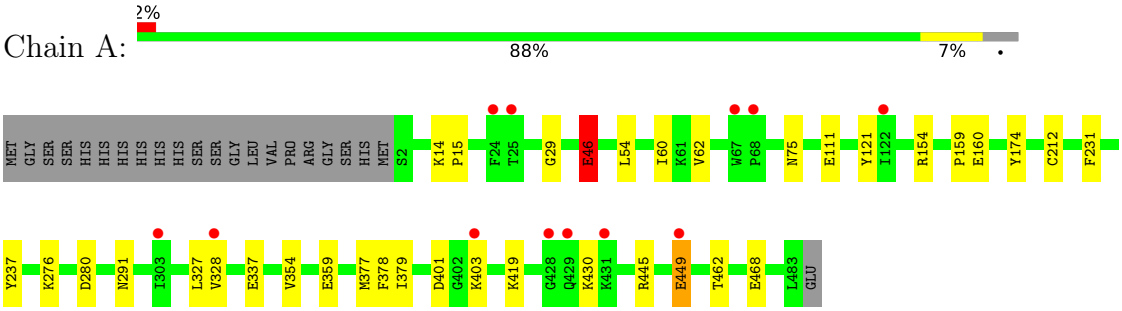
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	213	Total O 213 213	0	0
4	B	175	Total O 175 175	0	0
4	C	239	Total O 239 239	0	0
4	D	205	Total O 205 205	0	0
4	E	191	Total O 191 191	0	0
4	F	224	Total O 224 224	0	0

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.

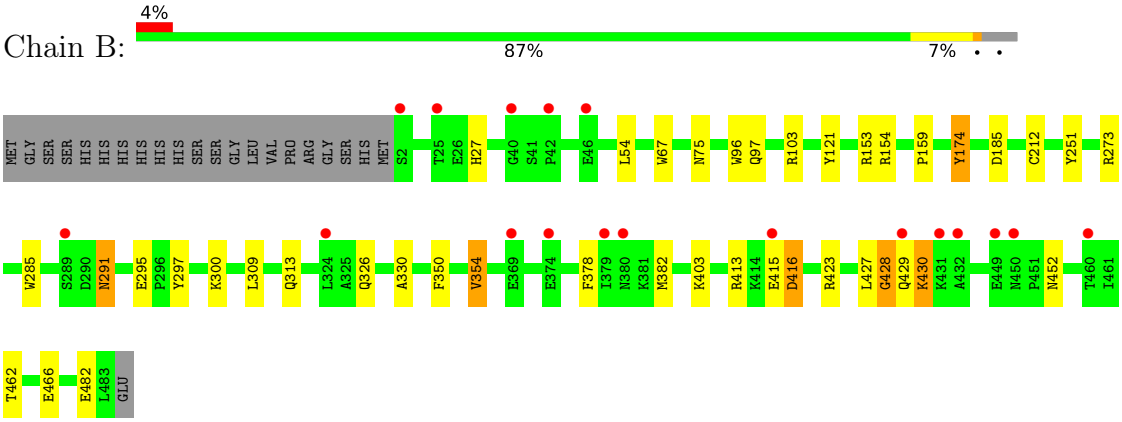
• Molecule 1: Alpha-L-arabinofuranosidase

Chain A:



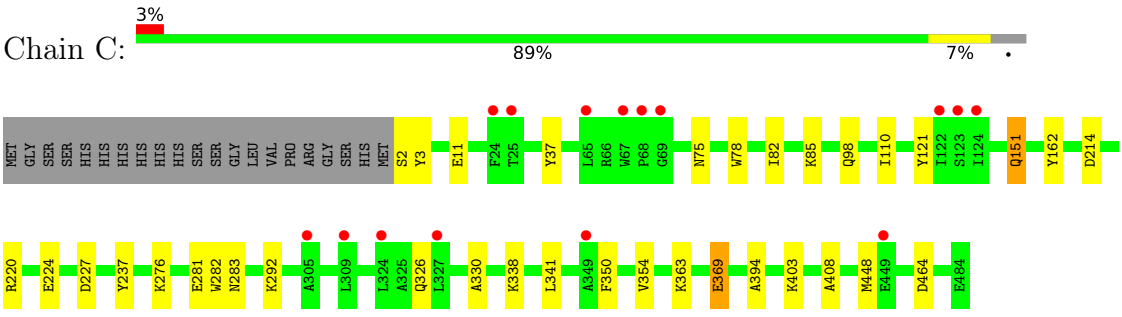
• Molecule 1: Alpha-L-arabinofuranosidase

Chain B:



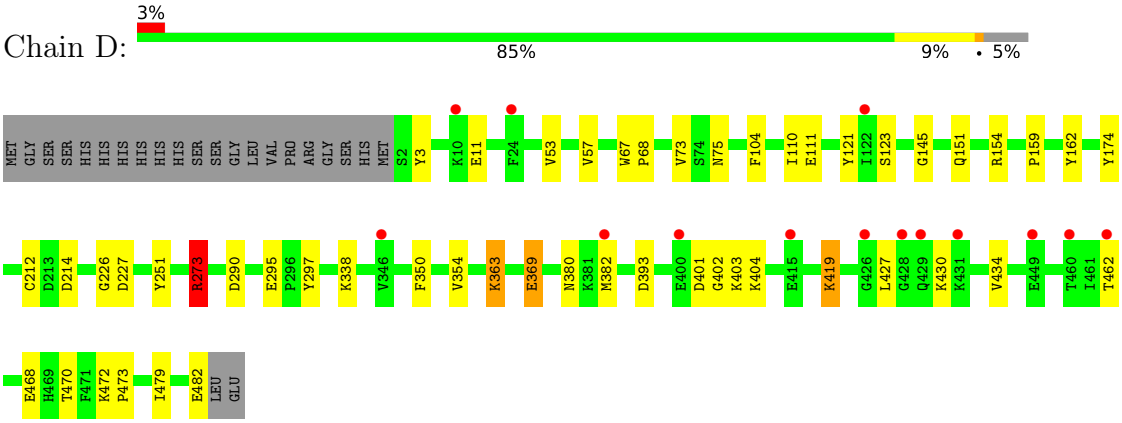
• Molecule 1: Alpha-L-arabinofuranosidase

Chain C:



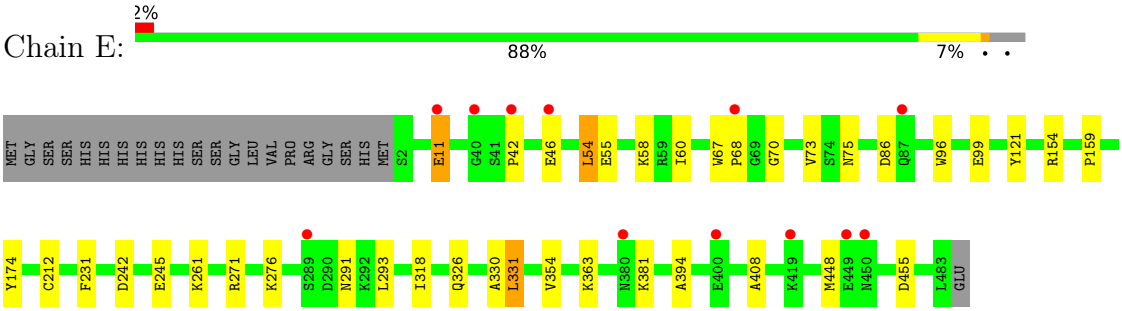
• Molecule 1: Alpha-L-arabinofuranosidase

Chain D:



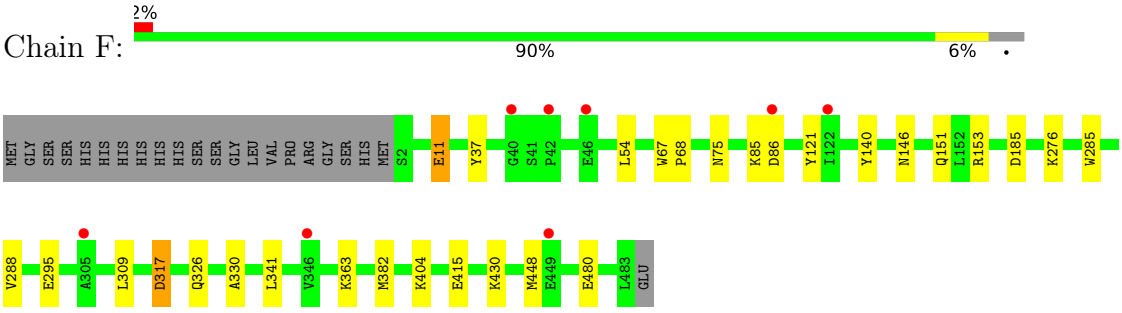
• Molecule 1: Alpha-L-arabinofuranosidase

Chain E:



• Molecule 1: Alpha-L-arabinofuranosidase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.20Å 160.93Å 156.17Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	29.59 – 2.30 29.59 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.59-2.30) 99.3 (29.59-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.168 , 0.209 0.165 , 0.204	Depositor DCC
R_{free} test set	11084 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.9	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.004 for -h,-l,-k 0.000 for -h,l,k 0.012 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	24750	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, TRS

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	1.04	7/3973 (0.2%)	0.86	3/5392 (0.1%)
1	B	1.05	1/3973 (0.0%)	0.89	7/5392 (0.1%)
1	C	1.03	3/3982 (0.1%)	0.85	4/5404 (0.1%)
1	D	1.04	3/3965 (0.1%)	0.85	3/5381 (0.1%)
1	E	0.98	3/3973 (0.1%)	0.84	4/5392 (0.1%)
1	F	0.98	0/3973	0.85	2/5392 (0.0%)
All	All	1.02	17/23839 (0.1%)	0.86	23/32353 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	46	GLU	CG-CD	8.16	1.64	1.51
1	A	46	GLU	CG-CD	7.68	1.63	1.51
1	C	98	GLN	CG-CD	6.80	1.66	1.51
1	A	160	GLU	CG-CD	6.32	1.61	1.51
1	A	449	GLU	CG-CD	6.29	1.61	1.51
1	E	46	GLU	CB-CG	6.02	1.63	1.52
1	E	55	GLU	CG-CD	5.82	1.60	1.51
1	A	62	VAL	CB-CG1	5.69	1.64	1.52
1	D	104	PHE	CE2-CZ	5.56	1.48	1.37
1	B	174	TYR	CD1-CE1	5.53	1.47	1.39
1	A	337	GLU	CG-CD	5.53	1.60	1.51
1	C	224	GLU	CB-CG	-5.29	1.42	1.52
1	D	111	GLU	CG-CD	5.24	1.59	1.51
1	A	46	GLU	CB-CG	5.18	1.61	1.52
1	C	151	GLN	CG-CD	5.07	1.62	1.51
1	A	359	GLU	CG-CD	5.03	1.59	1.51
1	D	151	GLN	CG-CD	5.00	1.62	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	273	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	B	185	ASP	CB-CG-OD1	6.91	124.52	118.30
1	F	317	ASP	CB-CG-OD1	6.51	124.16	118.30
1	D	290	ASP	CB-CG-OD1	6.39	124.06	118.30
1	B	54	LEU	CB-CG-CD1	-6.31	100.28	111.00
1	E	455	ASP	CB-CG-OD1	6.27	123.94	118.30
1	B	103	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	C	214	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	280	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	382	MET	CG-SD-CE	5.61	109.18	100.20
1	A	291	ASN	CB-CA-C	-5.46	99.47	110.40
1	C	220	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	227	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	464	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	B	67	TRP	C-N-CD	-5.33	108.87	120.60
1	B	153	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	54	LEU	CA-CB-CG	5.31	127.52	115.30
1	D	214	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	E	86	ASP	CB-CG-OD1	5.17	122.95	118.30
1	F	86	ASP	CB-CG-OD1	5.11	122.90	118.30
1	E	291	ASN	CB-CA-C	-5.10	100.21	110.40
1	B	251	TYR	CA-CB-CG	-5.04	103.82	113.40
1	E	271	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3876	0	3793	13	0
1	B	3876	0	3793	13	0
1	C	3885	0	3799	19	0
1	D	3868	0	3782	22	0
1	E	3876	0	3793	18	0
1	F	3876	0	3793	17	0
2	A	16	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	16	0	24	0	0
2	C	16	0	24	5	0
2	D	16	0	24	0	0
2	E	16	0	24	2	0
2	F	16	0	24	3	0
3	A	30	0	0	1	0
3	B	30	0	0	0	0
3	C	20	0	0	0	0
3	D	40	0	0	0	0
3	E	20	0	0	0	0
3	F	10	0	0	1	0
4	A	213	0	0	1	0
4	B	175	0	0	0	0
4	C	239	0	0	3	0
4	D	205	0	0	0	0
4	E	191	0	0	0	0
4	F	224	0	0	5	0
All	All	24750	0	22897	105	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 2.

All (105) 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)
2:C:486:TRS:H31	4:C:1244:HOH:O	1.69	0.92
1:C:237:TYR:OH	2:C:486:TRS:H21	1.75	0.86
1:F:11:GLU:HG2	1:F:363:LYS:HB2	1.60	0.84
1:F:185:ASP:HB3	4:F:1239:HOH:O	1.81	0.79
1:D:11:GLU:HG2	1:D:363:LYS:HD3	1.66	0.75
1:E:11:GLU:HG2	1:E:363:LYS:HB2	1.69	0.74
2:F:486:TRS:H21	4:F:1247:HOH:O	1.88	0.73
1:A:29:GLY:O	3:A:488:XYP:C5	2.38	0.71
1:D:419:LYS:HE2	1:D:468:GLU:OE1	1.93	0.68
1:C:237:TYR:HH	2:C:486:TRS:H21	1.60	0.66
1:F:151:GLN:HG2	4:F:497:HOH:O	1.95	0.66
1:B:350:PHE:O	1:B:354:VAL:HB	1.96	0.66
1:C:237:TYR:OH	2:C:486:TRS:C2	2.44	0.66
1:C:11:GLU:HG2	1:C:363:LYS:HE3	1.77	0.66
1:E:293:LEU:HB3	1:E:331:LEU:HD13	1.77	0.65
1:A:154:ARG:HG2	1:A:159:PRO:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:TYR:OH	2:A:486:TRS:H21	1.98	0.63
1:D:3:TYR:CZ	1:D:369:GLU:HG3	2.35	0.61
1:C:281:GLU:OE2	2:C:486:TRS:H21	2.01	0.59
1:D:295:GLU:HG2	1:D:297:TYR:CE1	2.38	0.59
1:B:96:TRP:HE3	1:B:291:ASN:HB3	1.68	0.58
1:B:326:GLN:HB2	1:B:330:ALA:O	2.03	0.58
2:A:486:TRS:H31	4:A:1245:HOH:O	2.04	0.58
1:E:96:TRP:HZ2	2:E:486:TRS:H21	1.70	0.57
1:E:11:GLU:HG2	1:E:363:LYS:CB	2.34	0.57
1:D:434:VAL:HG22	1:D:479:ILE:HG12	1.87	0.57
1:D:403:LYS:O	1:D:482:GLU:HG2	2.06	0.56
1:E:326:GLN:HB2	1:E:330:ALA:O	2.05	0.56
1:F:341:LEU:C	1:F:341:LEU:HD12	2.29	0.53
1:A:46:GLU:H	1:A:46:GLU:CD	2.13	0.52
1:C:3:TYR:OH	1:C:369:GLU:HG3	2.09	0.52
1:F:285:TRP:CZ3	2:F:486:TRS:O3	2.64	0.51
1:B:423:ARG:NH1	1:B:466:GLU:OE2	2.44	0.51
1:C:3:TYR:CZ	1:C:369:GLU:HG3	2.45	0.51
1:D:154:ARG:HG2	1:D:159:PRO:HA	1.92	0.49
1:B:96:TRP:CE3	1:B:291:ASN:HB3	2.47	0.49
1:F:37:TYR:OH	1:F:85:LYS:NZ	2.42	0.49
1:E:261:LYS:HG3	1:E:318:ILE:HG12	1.95	0.48
1:C:350:PHE:O	1:C:354:VAL:HB	2.13	0.48
1:D:226:GLY:O	1:D:273:ARG:HD3	2.14	0.48
1:F:382:MET:CE	4:F:1205:HOH:O	2.62	0.48
1:C:338:LYS:HG2	4:C:516:HOH:O	2.13	0.47
1:C:151:GLN:HG2	4:C:908:HOH:O	2.13	0.47
1:F:288:VAL:HG22	1:F:295:GLU:OE1	2.13	0.47
1:C:341:LEU:C	1:C:341:LEU:HD12	2.35	0.47
1:D:174:TYR:CE2	1:D:212:CYS:HB3	2.50	0.46
1:E:60:ILE:O	1:E:354:VAL:HG11	2.15	0.46
1:E:96:TRP:CZ2	2:E:486:TRS:H21	2.49	0.46
1:B:285:TRP:CE3	1:B:378:PHE:HE1	2.33	0.46
1:D:67:TRP:CE2	1:D:68:PRO:HB3	2.51	0.46
1:E:154:ARG:HG2	1:E:159:PRO:HA	1.97	0.46
1:D:472:LYS:HB3	1:D:473:PRO:HD2	1.98	0.45
1:E:394:ALA:HA	1:E:408:ALA:O	2.16	0.45
1:A:14:LYS:HB2	1:A:15:PRO:HD2	1.99	0.45
1:B:427:LEU:O	1:B:428:GLY:O	2.34	0.45
1:C:276:LYS:HA	1:C:276:LYS:HD3	1.80	0.45
1:A:419:LYS:HD3	1:A:468:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:ALA:HA	1:C:408:ALA:O	2.17	0.44
1:D:73:VAL:HG21	1:D:123:SER:O	2.18	0.44
1:C:37:TYR:OH	1:C:85:LYS:NZ	2.46	0.44
1:D:11:GLU:HG2	1:D:363:LYS:HB2	2.00	0.44
1:C:282:TRP:O	1:C:283:ASN:HB2	2.18	0.43
1:B:309:LEU:O	1:B:313:GLN:HG3	2.17	0.43
1:D:380:ASN:OD1	1:D:382:MET:HG3	2.17	0.43
1:F:404:LYS:NZ	1:F:480:GLU:OE2	2.52	0.43
1:A:60:ILE:O	1:A:354:VAL:HG21	2.18	0.43
1:D:419:LYS:HG2	1:D:470:THR:OG1	2.19	0.43
1:E:11:GLU:CG	1:E:363:LYS:HB2	2.42	0.43
1:E:231:PHE:HA	1:E:276:LYS:O	2.17	0.43
1:A:174:TYR:CE2	1:A:212:CYS:HB3	2.54	0.43
1:A:378:PHE:CG	1:A:379:ILE:N	2.87	0.43
1:B:300:LYS:HB3	1:B:300:LYS:HE3	1.73	0.43
1:F:276:LYS:HE3	1:F:317:ASP:O	2.18	0.43
1:D:350:PHE:O	1:D:354:VAL:HB	2.19	0.43
1:F:341:LEU:HD12	1:F:341:LEU:O	2.19	0.43
1:A:327:LEU:HG	1:A:328:VAL:HG23	2.00	0.43
1:B:154:ARG:HG2	1:B:159:PRO:HA	1.99	0.43
1:B:295:GLU:HG2	1:B:297:TYR:CE1	2.54	0.43
1:D:227:ASP:O	1:D:273:ARG:HD2	2.19	0.42
1:D:251:TYR:OH	1:D:393:ASP:OD2	2.33	0.42
1:A:401:ASP:OD1	1:A:403:LYS:HB2	2.20	0.42
1:E:70:GLY:O	1:E:73:VAL:HG12	2.19	0.42
2:F:486:TRS:H31	3:F:487:XYP:O2	2.19	0.42
1:F:382:MET:HE1	4:F:1205:HOH:O	2.19	0.42
1:C:403:LYS:HA	1:C:403:LYS:HD3	1.92	0.42
1:E:242:ASP:HB3	1:E:245:GLU:HB2	2.02	0.42
1:F:67:TRP:CE2	1:F:68:PRO:HB3	2.54	0.42
1:F:309:LEU:HD23	1:F:309:LEU:HA	1.92	0.42
1:D:401:ASP:OD1	1:D:402:GLY:N	2.53	0.42
1:E:67:TRP:CE2	1:E:68:PRO:HB3	2.55	0.42
1:F:326:GLN:HB2	1:F:330:ALA:O	2.20	0.42
1:E:174:TYR:CE2	1:E:212:CYS:HB3	2.55	0.41
1:A:231:PHE:HA	1:A:276:LYS:O	2.19	0.41
1:C:326:GLN:HB2	1:C:330:ALA:O	2.20	0.41
1:E:54:LEU:O	1:E:58:LYS:HG3	2.21	0.41
1:D:53:VAL:O	1:D:57:VAL:HG23	2.20	0.41
1:D:110:ILE:HG21	1:D:162:TYR:CD1	2.56	0.41
1:B:415:GLU:HB2	1:B:416:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:TRP:CD1	1:F:68:PRO:HA	2.56	0.41
1:B:174:TYR:CE2	1:B:212:CYS:HB3	2.56	0.41
1:C:78:TRP:CZ3	1:C:82:ILE:HD13	2.56	0.40
1:A:377:MET:O	1:A:378:PHE:HB3	2.21	0.40
1:C:110:ILE:HG21	1:C:162:TYR:CD1	2.56	0.40
1:D:145:GLY:HA3	1:E:99:GLU:OE2	2.21	0.40
1:F:140:TYR:O	1:F:153:ARG:HD3	2.20	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	480/504 (95%)	463 (96%)	17 (4%)	0	100 100
1	B	480/504 (95%)	453 (94%)	24 (5%)	3 (1%)	25 31
1	C	481/504 (95%)	464 (96%)	17 (4%)	0	100 100
1	D	479/504 (95%)	452 (94%)	27 (6%)	0	100 100
1	E	480/504 (95%)	463 (96%)	17 (4%)	0	100 100
1	F	480/504 (95%)	452 (94%)	28 (6%)	0	100 100
All	All	2880/3024 (95%)	2747 (95%)	130 (4%)	3 (0%)	51 64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	428	GLY
1	B	27	HIS
1	B	430	LYS

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	417/436 (96%)	409 (98%)	8 (2%)	57	73
1	B	417/436 (96%)	403 (97%)	14 (3%)	37	51
1	C	418/436 (96%)	412 (99%)	6 (1%)	67	81
1	D	416/436 (95%)	405 (97%)	11 (3%)	46	63
1	E	417/436 (96%)	409 (98%)	8 (2%)	57	73
1	F	417/436 (96%)	409 (98%)	8 (2%)	57	73
All	All	2502/2616 (96%)	2447 (98%)	55 (2%)	52	69

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLU
1	A	75	ASN
1	A	111	GLU
1	A	121	TYR
1	A	430	LYS
1	A	445	ARG
1	A	449	GLU
1	A	462	THR
1	B	75	ASN
1	B	97	GLN
1	B	121	TYR
1	B	273	ARG
1	B	291	ASN
1	B	354	VAL
1	B	403	LYS
1	B	413	ARG
1	B	416	ASP
1	B	429	GLN
1	B	430	LYS
1	B	452	ASN
1	B	462	THR
1	B	482	GLU

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Mol	Chain	Res	Type
1	C	2	SER
1	C	75	ASN
1	C	121	TYR
1	C	292	LYS
1	C	369	GLU
1	C	448	MET
1	D	75	ASN
1	D	121	TYR
1	D	273	ARG
1	D	338	LYS
1	D	363	LYS
1	D	369	GLU
1	D	404	LYS
1	D	419	LYS
1	D	427	LEU
1	D	430	LYS
1	D	462	THR
1	E	11	GLU
1	E	42	PRO
1	E	54	LEU
1	E	75	ASN
1	E	121	TYR
1	E	331	LEU
1	E	381	LYS
1	E	448	MET
1	F	11	GLU
1	F	54	LEU
1	F	75	ASN
1	F	121	TYR
1	F	146	ASN
1	F	415	GLU
1	F	430	LYS
1	F	448	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

27 ligands 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	TRS	A	486	-	7,7,7	0.33	0	9,9,9	1.38	2 (22%)
2	TRS	C	485	-	7,7,7	0.73	0	9,9,9	1.51	1 (11%)
2	TRS	B	486	-	7,7,7	0.27	0	9,9,9	1.51	2 (22%)
3	XYP	D	490	-	10,10,10	1.94	4 (40%)	14,14,14	1.87	3 (21%)
2	TRS	F	485	-	7,7,7	0.35	0	9,9,9	0.65	0
3	XYP	D	488	-	10,10,10	2.63	3 (30%)	14,14,14	1.46	3 (21%)
3	XYP	B	489	-	10,10,10	2.74	5 (50%)	14,14,14	1.49	2 (14%)
3	XYP	B	488	-	10,10,10	2.45	3 (30%)	14,14,14	3.09	9 (64%)
3	XYP	B	487	-	10,10,10	1.12	1 (10%)	14,14,14	0.48	0
3	XYP	F	487	-	10,10,10	2.03	2 (20%)	14,14,14	1.34	2 (14%)
2	TRS	F	486	-	7,7,7	0.43	0	9,9,9	1.57	2 (22%)
3	XYP	E	487	-	10,10,10	1.94	1 (10%)	14,14,14	1.62	3 (21%)
2	TRS	A	485	-	7,7,7	0.35	0	9,9,9	0.62	0
2	TRS	B	485	-	7,7,7	0.47	0	9,9,9	1.09	0
2	TRS	E	486	-	7,7,7	0.30	0	9,9,9	1.02	0
3	XYP	E	488	-	10,10,10	2.61	4 (40%)	14,14,14	2.34	7 (50%)
3	XYP	D	489	-	10,10,10	2.32	4 (40%)	14,14,14	2.22	3 (21%)
3	XYP	A	487	-	10,10,10	1.29	1 (10%)	14,14,14	1.38	3 (21%)
2	TRS	E	485	-	7,7,7	0.58	0	9,9,9	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	TRS	D	485	-	7,7,7	0.29	0	9,9,9	0.97	0
3	XYP	A	489	-	10,10,10	2.99	4 (40%)	14,14,14	2.45	5 (35%)
3	XYP	D	487	-	10,10,10	2.26	4 (40%)	14,14,14	1.27	2 (14%)
3	XYP	C	487	-	10,10,10	1.48	1 (10%)	14,14,14	1.30	2 (14%)
3	XYP	A	488	-	10,10,10	4.29	5 (50%)	14,14,14	3.61	5 (35%)
2	TRS	C	486	-	7,7,7	0.59	0	9,9,9	1.08	0
2	TRS	D	486	-	7,7,7	0.46	0	9,9,9	1.21	1 (11%)
3	XYP	C	488	-	10,10,10	2.61	3 (30%)	14,14,14	2.20	6 (42%)

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	TRS	A	486	-	-	6/9/9/9	-
2	TRS	C	485	-	-	0/9/9/9	-
2	TRS	B	486	-	-	6/9/9/9	-
3	XYP	D	490	-	-	-	0/1/1/1
2	TRS	F	485	-	-	1/9/9/9	-
3	XYP	D	488	-	-	-	0/1/1/1
3	XYP	B	489	-	-	-	0/1/1/1
3	XYP	B	488	-	-	-	0/1/1/1
3	XYP	B	487	-	-	-	0/1/1/1
3	XYP	F	487	-	-	-	0/1/1/1
2	TRS	F	486	-	-	6/9/9/9	-
3	XYP	E	487	-	-	-	0/1/1/1
2	TRS	A	485	-	-	0/9/9/9	-
2	TRS	B	485	-	-	0/9/9/9	-
2	TRS	E	486	-	-	6/9/9/9	-
3	XYP	E	488	-	-	-	0/1/1/1
3	XYP	D	489	-	-	-	0/1/1/1
3	XYP	A	487	-	-	-	0/1/1/1
2	TRS	E	485	-	-	0/9/9/9	-
2	TRS	D	485	-	-	0/9/9/9	-
3	XYP	A	489	-	-	-	0/1/1/1
3	XYP	D	487	-	-	-	0/1/1/1
3	XYP	C	487	-	-	-	0/1/1/1
3	XYP	A	488	-	-	-	0/1/1/1
2	TRS	C	486	-	-	8/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	D	486	-	-	6/9/9/9	-
3	XYP	C	488	-	-	-	0/1/1/1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	488	XYP	C4-C3	7.73	1.63	1.52
3	A	488	XYP	O4-C4	7.20	1.58	1.43
3	B	489	XYP	O5-C1	6.61	1.52	1.43
3	A	489	XYP	O5-C1	6.57	1.52	1.43
3	A	488	XYP	O5-C5	6.48	1.54	1.43
3	D	488	XYP	O5-C1	6.21	1.51	1.43
3	C	488	XYP	O5-C1	6.04	1.51	1.43
3	D	489	XYP	O5-C1	5.49	1.50	1.43
3	E	488	XYP	C4-C3	5.49	1.60	1.52
3	A	489	XYP	C4-C3	5.34	1.60	1.52
3	F	487	XYP	O5-C1	5.02	1.50	1.43
3	E	487	XYP	O5-C1	4.98	1.50	1.43
3	B	488	XYP	C4-C3	4.88	1.59	1.52
3	E	488	XYP	O5-C1	4.43	1.49	1.43
3	B	488	XYP	O2-C2	4.38	1.53	1.43
3	A	488	XYP	O5-C1	4.34	1.49	1.43
3	D	487	XYP	O5-C5	4.26	1.50	1.43
3	D	487	XYP	O5-C1	4.10	1.48	1.43
3	C	488	XYP	O5-C5	3.46	1.49	1.43
3	D	490	XYP	O1-C1	3.41	1.50	1.39
3	C	488	XYP	C4-C3	3.21	1.57	1.52
3	C	487	XYP	O5-C1	3.00	1.47	1.43
3	B	488	XYP	O5-C1	2.95	1.47	1.43
3	F	487	XYP	O5-C5	2.94	1.48	1.43
3	D	489	XYP	O5-C5	2.87	1.48	1.43
3	D	488	XYP	C4-C3	2.82	1.56	1.52
3	D	490	XYP	O3-C3	2.69	1.49	1.43
3	D	488	XYP	O1-C1	2.64	1.48	1.39
3	B	489	XYP	C4-C3	2.62	1.56	1.52
3	D	487	XYP	O1-C1	2.60	1.47	1.39
3	D	490	XYP	O5-C1	2.60	1.46	1.43
3	D	489	XYP	C4-C3	2.55	1.56	1.52
3	E	488	XYP	O5-C5	2.39	1.47	1.43
3	B	489	XYP	O1-C1	2.38	1.47	1.39
3	B	489	XYP	C1-C2	2.38	1.58	1.52
3	B	487	XYP	O5-C5	2.31	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	487	XYP	C4-C3	2.19	1.55	1.52
3	A	489	XYP	C1-C2	2.19	1.57	1.52
3	A	487	XYP	O5-C1	2.18	1.46	1.43
3	E	488	XYP	C5-C4	2.11	1.57	1.52
3	B	489	XYP	O5-C5	2.10	1.47	1.43
3	D	490	XYP	C1-C2	2.10	1.57	1.52
3	A	488	XYP	C3-C2	2.10	1.57	1.52
3	D	489	XYP	C1-C2	2.06	1.57	1.52
3	A	489	XYP	O1-C1	2.05	1.46	1.39

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	488	XYP	O5-C5-C4	10.77	127.39	110.77
3	A	488	XYP	O4-C4-C3	5.29	120.74	110.14
3	B	488	XYP	C1-C2-C3	-5.24	99.45	110.31
3	B	488	XYP	O1-C1-C2	4.71	122.29	109.03
3	D	490	XYP	O5-C5-C4	4.58	117.85	110.77
3	D	489	XYP	O5-C5-C4	4.56	117.81	110.77
3	D	489	XYP	O5-C1-C2	4.50	116.11	109.43
3	E	488	XYP	C1-C2-C3	-4.49	100.99	110.31
3	B	488	XYP	O2-C2-C1	4.46	119.51	109.16
3	C	488	XYP	O5-C5-C4	4.45	117.64	110.77
3	A	489	XYP	O3-C3-C4	4.42	118.45	109.99
3	E	488	XYP	O3-C3-C4	4.15	117.94	109.99
3	A	489	XYP	O5-C1-C2	4.11	115.53	109.43
3	D	489	XYP	C5-O5-C1	4.01	119.46	112.71
3	B	488	XYP	O2-C2-C3	4.00	119.61	110.35
3	E	487	XYP	C5-C4-C3	3.96	114.54	109.67
3	A	489	XYP	O4-C4-C3	3.93	118.02	110.14
3	A	488	XYP	O3-C3-C4	3.75	117.17	109.99
3	B	489	XYP	O5-C1-C2	3.45	114.56	109.43
3	B	489	XYP	C5-C4-C3	3.42	113.87	109.67
3	D	490	XYP	O1-C1-C2	3.33	118.40	109.03
3	C	488	XYP	O5-C1-C2	3.32	114.37	109.43
3	A	489	XYP	C5-O5-C1	3.27	118.21	112.71
3	E	488	XYP	O4-C4-C3	3.23	116.61	110.14
3	F	487	XYP	O1-C1-O5	3.22	118.10	109.72
3	B	488	XYP	O3-C3-C4	3.19	116.11	109.99
3	C	488	XYP	C5-C4-C3	3.18	113.58	109.67
3	C	487	XYP	C5-O5-C1	3.16	118.02	112.71
3	B	488	XYP	O4-C4-C3	3.12	116.39	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	488	XYP	O1-C1-O5	-3.03	101.83	109.72
3	C	488	XYP	C1-C2-C3	-3.02	104.05	110.31
3	A	488	XYP	O1-C1-O5	2.98	117.48	109.72
2	C	485	TRS	C3-C-C2	-2.97	101.60	110.81
2	F	486	TRS	C3-C-C1	-2.95	101.67	110.81
3	D	487	XYP	C5-O5-C1	2.81	117.44	112.71
2	A	486	TRS	O1-C1-C	-2.80	102.12	111.00
3	D	488	XYP	C5-O5-C1	-2.79	108.01	112.71
3	A	487	XYP	C5-C4-C3	2.72	113.01	109.67
2	F	486	TRS	O1-C1-C	2.70	119.54	111.00
3	B	488	XYP	O5-C5-C4	-2.61	106.74	110.77
3	A	489	XYP	C4-C3-C2	-2.59	106.42	110.89
3	A	487	XYP	O4-C4-C3	-2.52	105.09	110.14
3	D	490	XYP	C5-C4-C3	2.51	112.75	109.67
2	B	486	TRS	O1-C1-C	-2.39	103.42	111.00
3	E	488	XYP	O2-C2-C1	2.38	114.68	109.16
3	D	488	XYP	C5-C4-C3	2.34	112.55	109.67
2	A	486	TRS	C2-C-C1	-2.33	103.59	110.81
3	E	488	XYP	O2-C2-C3	2.31	115.68	110.35
3	C	487	XYP	O4-C4-C3	-2.29	105.56	110.14
3	A	487	XYP	C5-O5-C1	2.25	116.50	112.71
2	B	486	TRS	C3-C-C1	-2.22	103.94	110.81
3	A	488	XYP	C5-C4-C3	-2.15	107.02	109.67
3	E	487	XYP	O1-C1-C2	2.15	115.09	109.03
3	C	488	XYP	O3-C3-C4	2.13	114.07	109.99
3	D	487	XYP	O1-C1-C2	2.12	114.99	109.03
3	E	488	XYP	O5-C5-C4	2.10	114.02	110.77
2	D	486	TRS	C2-C-N	2.10	114.24	107.98
3	B	488	XYP	C4-C3-C2	-2.06	107.33	110.89
3	E	488	XYP	C5-C4-C3	2.04	112.17	109.67
3	D	488	XYP	O1-C1-O5	2.03	115.01	109.72
3	E	487	XYP	C5-O5-C1	2.01	116.09	112.71
3	C	488	XYP	O1-C1-O5	2.00	114.94	109.72
3	F	487	XYP	O4-C4-C5	2.00	113.25	109.15

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	486	TRS	C1-C-C2-O2
2	A	486	TRS	C3-C-C2-O2
2	A	486	TRS	N-C-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	486	TRS	C1-C-C3-O3
2	A	486	TRS	C2-C-C3-O3
2	A	486	TRS	N-C-C3-O3
2	B	486	TRS	C1-C-C2-O2
2	C	486	TRS	N-C-C1-O1
2	C	486	TRS	C1-C-C3-O3
2	C	486	TRS	C2-C-C3-O3
2	C	486	TRS	N-C-C3-O3
2	D	486	TRS	N-C-C1-O1
2	D	486	TRS	C1-C-C2-O2
2	D	486	TRS	C3-C-C2-O2
2	D	486	TRS	N-C-C2-O2
2	E	486	TRS	N-C-C1-O1
2	E	486	TRS	N-C-C2-O2
2	F	486	TRS	C2-C-C1-O1
2	F	486	TRS	C3-C-C1-O1
2	F	486	TRS	N-C-C1-O1
2	F	486	TRS	C1-C-C2-O2
2	F	486	TRS	C3-C-C2-O2
2	F	486	TRS	N-C-C2-O2
2	C	486	TRS	C3-C-C2-O2
2	D	486	TRS	C3-C-C1-O1
2	E	486	TRS	C3-C-C1-O1
2	E	486	TRS	C1-C-C2-O2
2	B	486	TRS	N-C-C2-O2
2	C	486	TRS	N-C-C2-O2
2	E	486	TRS	C2-C-C1-O1
2	B	486	TRS	C3-C-C2-O2
2	B	486	TRS	C2-C-C3-O3
2	C	486	TRS	C2-C-C1-O1
2	C	486	TRS	C1-C-C2-O2
2	D	486	TRS	C2-C-C1-O1
2	E	486	TRS	C3-C-C2-O2
2	B	486	TRS	C1-C-C3-O3
2	B	486	TRS	N-C-C3-O3
2	F	485	TRS	C3-C-C2-O2

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	486	TRS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	487	XYP	1	0
2	F	486	TRS	3	0
2	E	486	TRS	2	0
3	A	488	XYP	1	0
2	C	486	TRS	5	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, 95^{th} 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	482/504 (95%)	-0.20	12 (2%)	57	64	21, 30, 50, 63	0
1	B	482/504 (95%)	-0.09	18 (3%)	41	48	23, 33, 52, 66	0
1	C	483/504 (95%)	-0.18	15 (3%)	49	56	21, 30, 48, 64	0
1	D	481/504 (95%)	-0.20	14 (2%)	51	58	22, 32, 50, 65	0
1	E	482/504 (95%)	-0.25	12 (2%)	57	64	23, 32, 50, 64	0
1	F	482/504 (95%)	-0.24	8 (1%)	70	76	23, 32, 49, 64	0
All	All	2892/3024 (95%)	-0.19	79 (2%)	54	62	21, 32, 50, 66	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	449	GLU	4.7
1	D	431	LYS	4.3
1	D	429	GLN	4.2
1	D	449	GLU	4.0
1	B	431	LYS	3.8
1	F	449	GLU	3.8
1	A	428	GLY	3.6
1	C	449	GLU	3.5
1	E	449	GLU	3.4
1	C	324	LEU	3.4
1	E	46	GLU	3.3
1	B	460	THR	3.2
1	B	429	GLN	3.1
1	B	2	SER	3.1
1	A	449	GLU	3.1
1	F	46	GLU	3.1
1	C	68	PRO	3.0
1	C	327	LEU	2.9
1	D	382	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	25	THR	2.9
1	C	67	TRP	2.9
1	D	460	THR	2.8
1	C	305	ALA	2.8
1	A	429	GLN	2.8
1	D	462	THR	2.8
1	B	415	GLU	2.7
1	A	68	PRO	2.7
1	B	42	PRO	2.6
1	F	42	PRO	2.6
1	B	289	SER	2.5
1	E	68	PRO	2.5
1	C	24	PHE	2.5
1	A	25	THR	2.5
1	D	10	LYS	2.5
1	C	349	ALA	2.5
1	A	24	PHE	2.5
1	C	122	ILE	2.5
1	B	324	LEU	2.5
1	C	123	SER	2.4
1	E	40	GLY	2.4
1	C	124	ILE	2.4
1	F	40	GLY	2.4
1	D	24	PHE	2.4
1	A	67	TRP	2.3
1	C	309	LEU	2.3
1	E	87	GLN	2.3
1	D	426	GLY	2.3
1	B	380	ASN	2.3
1	B	432	ALA	2.3
1	E	11	GLU	2.3
1	E	42	PRO	2.3
1	E	380	ASN	2.3
1	E	400	GLU	2.3
1	B	25	THR	2.2
1	B	379	ILE	2.2
1	F	305	ALA	2.2
1	D	415	GLU	2.2
1	A	303	ILE	2.2
1	B	46	GLU	2.2
1	A	328	VAL	2.2
1	B	40	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	65	LEU	2.1
1	A	431	LYS	2.1
1	D	122	ILE	2.1
1	B	369	GLU	2.1
1	A	403	LYS	2.1
1	B	374	GLU	2.1
1	E	419	LYS	2.1
1	F	122	ILE	2.1
1	B	450	ASN	2.1
1	E	450	ASN	2.0
1	D	428	GLY	2.0
1	F	346	VAL	2.0
1	D	400	GLU	2.0
1	F	86	ASP	2.0
1	D	346	VAL	2.0
1	A	122	ILE	2.0
1	C	69	GLY	2.0
1	E	289	SER	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)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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
3	XYP	E	488	10/10	0.72	0.29	64,75,77,79	0
3	XYP	A	488	10/10	0.76	0.21	44,55,58,59	0
3	XYP	D	488	10/10	0.77	0.28	51,61,67,69	0
3	XYP	C	488	10/10	0.77	0.28	68,73,76,77	0
3	XYP	A	489	10/10	0.78	0.21	52,59,60,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TRS	C	486	8/8	0.85	0.20	45,50,51,52	0
3	XYP	B	489	10/10	0.86	0.18	62,68,70,71	0
3	XYP	B	488	10/10	0.87	0.20	43,56,59,64	0
3	XYP	D	490	10/10	0.89	0.22	54,60,61,63	0
2	TRS	F	486	8/8	0.91	0.18	51,53,54,55	0
3	XYP	D	489	10/10	0.91	0.23	55,60,62,65	0
2	TRS	E	486	8/8	0.92	0.18	47,48,51,51	0
3	XYP	C	487	10/10	0.93	0.13	44,48,49,52	0
3	XYP	E	487	10/10	0.93	0.10	43,46,49,49	0
2	TRS	A	486	8/8	0.93	0.14	41,45,46,48	0
2	TRS	D	486	8/8	0.94	0.18	34,39,42,43	0
2	TRS	B	486	8/8	0.94	0.14	42,43,45,46	0
3	XYP	D	487	10/10	0.95	0.09	43,47,49,51	0
3	XYP	A	487	10/10	0.95	0.11	38,40,41,41	0
3	XYP	B	487	10/10	0.95	0.08	44,47,48,48	0
3	XYP	F	487	10/10	0.95	0.13	49,50,53,53	0
2	TRS	C	485	8/8	0.98	0.09	22,25,27,28	0
2	TRS	F	485	8/8	0.98	0.08	32,32,33,33	0
2	TRS	B	485	8/8	0.98	0.09	27,29,29,31	0
2	TRS	D	485	8/8	0.98	0.07	28,30,31,31	0
2	TRS	A	485	8/8	0.98	0.08	28,30,32,32	0
2	TRS	E	485	8/8	0.98	0.09	31,32,33,34	0

6.5 Other polymers (i)

There are no such residues in this entry.