



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:40 PM UTC

PDB ID : 3UG5 / pdb_00003ug5
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.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

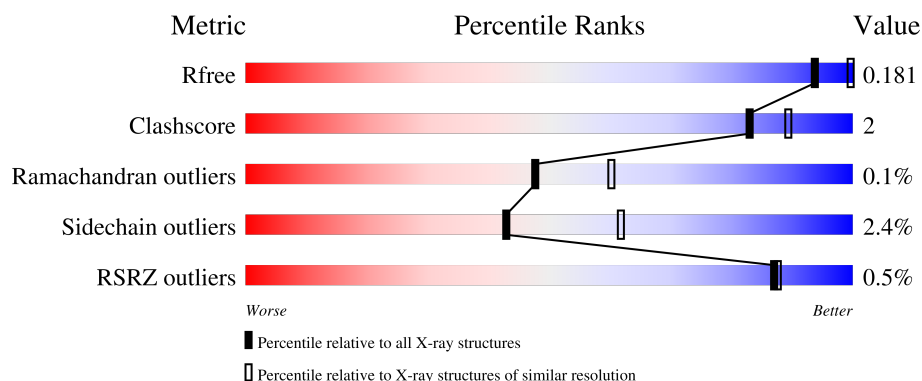
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	504	% 89% 6%
1	B	504	% 87% 8%
1	C	504	 89% 6%
1	D	504	% 84% 11%
1	E	504	 88% 7%

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Mol	Chain	Length	Quality of chain
1	F	504	% 89% 6% . .

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
2	TRS	A	486	-	X	-	-
2	TRS	F	486	-	X	-	-

2 Entry composition

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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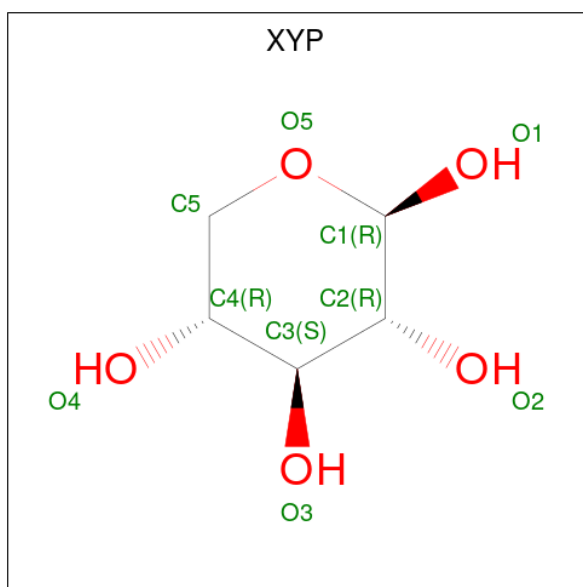
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q9WYB7
E	-1	SER	-	expression tag	UNP Q9WYB7
E	0	HIS	-	expression tag	UNP Q9WYB7
E	4	GLY	ARG	engineered mutation	UNP Q9WYB7
F	-19	MET	-	expression tag	UNP Q9WYB7
F	-18	GLY	-	expression tag	UNP Q9WYB7
F	-17	SER	-	expression tag	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 (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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 (CCD ID: XYP) (formula: C₅H₁₀O₅).



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

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

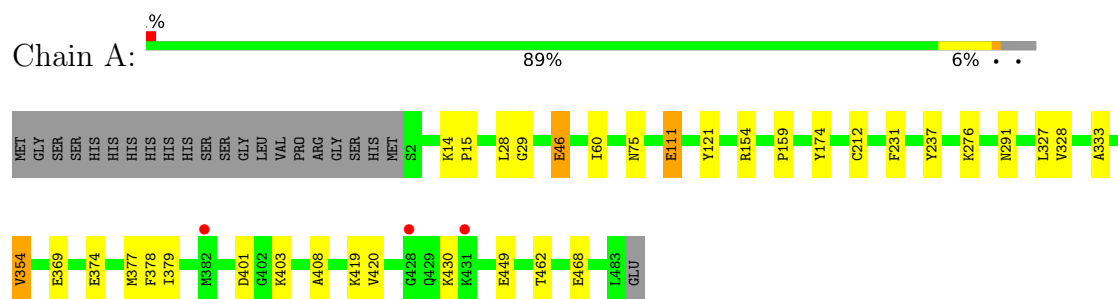
- Molecule 4 is water.

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

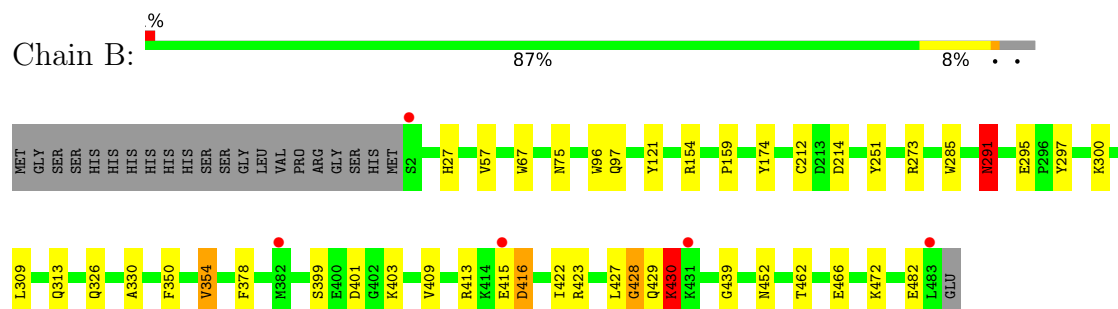
3 Residue-property plots [i](#)

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.

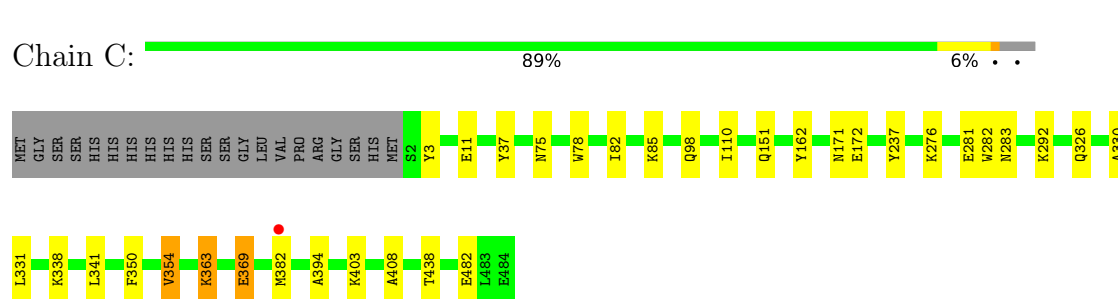
- Molecule 1: Alpha-L-arabinofuranosidase



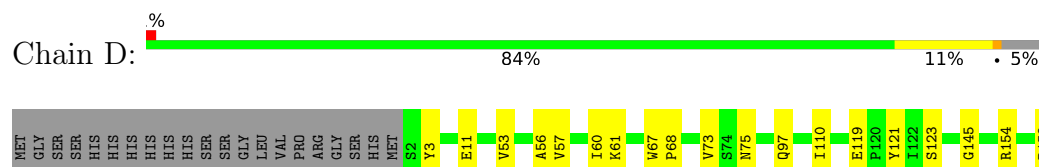
- Molecule 1: Alpha-L-arabinofuranosidase

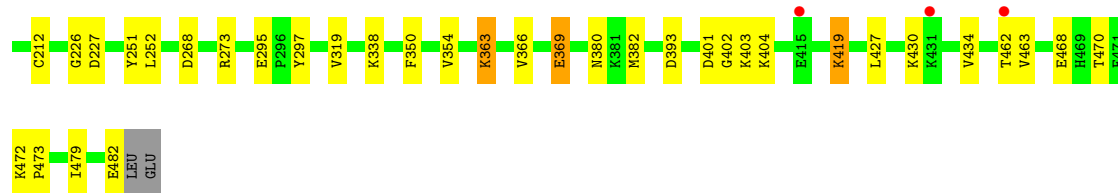


- Molecule 1: Alpha-L-arabinofuranosidase



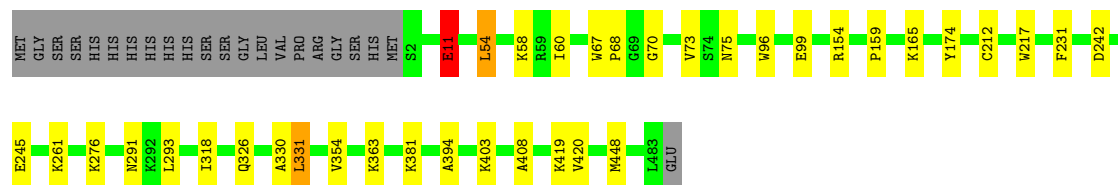
- Molecule 1: Alpha-L-arabinofuranosidase





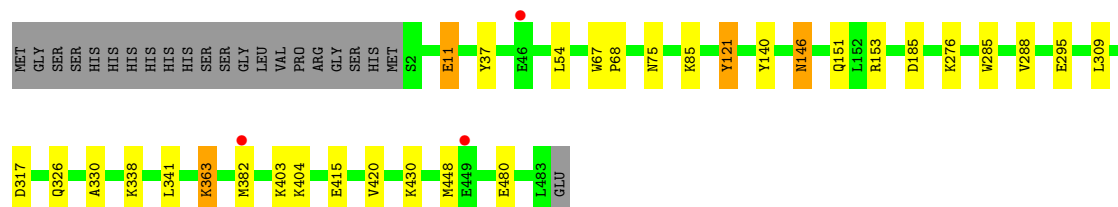
• Molecule 1: Alpha-L-arabinofuranosidase

Chain E: 88% 7% .



• Molecule 1: Alpha-L-arabinofuranosidase

Chain F: 89% 6% . .



4 Data and refinement statistics

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) 99.2 (29.59-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.168 , 0.209 (Not available) , 0.181	Depositor DCC
R_{free} test set	11084 reflections (4.98%)	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 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, XYP

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	1.17	3/3973 (0.1%)	1.05	3/5392 (0.1%)
1	B	1.19	4/3973 (0.1%)	1.11	8/5392 (0.1%)
1	C	1.16	2/3982 (0.1%)	1.03	0/5404
1	D	1.18	3/3965 (0.1%)	1.07	4/5381 (0.1%)
1	E	1.12	2/3973 (0.1%)	1.04	3/5392 (0.1%)
1	F	1.13	0/3973	1.05	2/5392 (0.0%)
All	All	1.16	14/23839 (0.1%)	1.06	20/32353 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	420	VAL	CA-CB	8.05	1.61	1.54
1	A	333	ALA	CA-CB	-6.36	1.43	1.53
1	C	98	GLN	CG-CD	5.85	1.66	1.52
1	B	409	VAL	CA-CB	5.62	1.62	1.54
1	D	56	ALA	CA-C	5.33	1.59	1.52
1	C	438	THR	CA-CB	5.30	1.60	1.53
1	B	430	LYS	N-CA	5.28	1.52	1.46
1	D	366	VAL	CA-CB	5.18	1.60	1.54
1	A	354	VAL	CA-CB	5.18	1.61	1.54
1	A	408	ALA	CA-CB	5.16	1.60	1.53
1	E	11	GLU	CA-C	5.14	1.59	1.52
1	B	422	ILE	CA-CB	5.07	1.60	1.54
1	D	319	VAL	CA-C	5.06	1.58	1.52
1	B	214	ASP	N-CA	-5.05	1.40	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	146	ASN	N-CA-C	7.25	120.99	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	472	LYS	CA-C-N	-6.50	113.94	120.31
1	B	472	LYS	C-N-CA	-6.50	113.94	120.31
1	F	420	VAL	N-CA-C	6.26	114.86	107.73
1	B	439	GLY	CA-C-N	6.08	125.80	119.05
1	B	439	GLY	C-N-CA	6.08	125.80	119.05
1	A	291	ASN	CB-CA-C	-5.85	99.47	110.01
1	B	57	VAL	N-CA-C	5.61	115.81	110.53
1	B	251	TYR	CA-CB-CG	-5.60	103.82	113.90
1	E	403	LYS	N-CA-C	5.57	120.08	113.28
1	D	119	GLU	CA-C-N	-5.45	114.34	119.85
1	D	119	GLU	C-N-CA	-5.45	114.34	119.85
1	E	291	ASN	CB-CA-C	-5.45	100.21	110.01
1	E	420	VAL	N-CA-C	5.45	116.31	107.71
1	B	291	ASN	N-CA-C	5.42	119.42	112.26
1	A	420	VAL	N-CA-C	5.42	113.80	107.89
1	B	67	TRP	C-N-CD	-5.33	108.87	120.60
1	D	252	LEU	N-CA-C	-5.27	104.97	111.40
1	A	111	GLU	N-CA-C	-5.08	105.74	111.28
1	D	268	ASP	N-CA-C	5.00	117.11	111.11

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	3876	0	3793	15	0
1	B	3876	0	3793	14	0
1	C	3885	0	3799	21	0
1	D	3868	0	3782	23	0
1	E	3876	0	3793	19	0
1	F	3876	0	3793	18	0
2	A	16	0	24	3	0
2	B	16	0	24	0	0
2	C	16	0	24	5	0
2	D	16	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	113	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 (113) 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:C:237:TYR:HH	2:C:486:TRS:H21	1.53	0.72
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:341:LEU:C	1:F:341:LEU:HD12	2.29	0.57
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:A:46:GLU:H	1:A:46:GLU:CD	2.13	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:C:3:TYR:OH	1:C:369:GLU:HG3	2.09	0.52
1:C:341:LEU:C	1:C:341:LEU:HD12	2.35	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: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:A:237:TYR:HH	2:A:486:TRS:H21	1.80	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:330:ALA:O	1:C:331:LEU:C	2.62	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:C:171:ASN:O	1:C:172:GLU:C	2.62	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:E:217:TRP:C	1:E:217:TRP:CD1	2.96	0.42
1:C:37:TYR:OH	1:C:85:LYS:NZ	2.46	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:28:LEU:O	1:A:29:GLY:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ILE:HG21	1:D:162:TYR:CD1	2.56	0.41
1:B:399:SER:OG	1:B:401:ASP:OD1	2.35	0.41
1:B:415:GLU:HB2	1:B:416:ASP:OD2	2.21	0.41
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:D:60:ILE:O	1:D:61:LYS:C	2.64	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:121:TYR:C	1:F:121:TYR:CD1	2.99	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	480/504 (95%)	463 (96%)	17 (4%)	0	100	100
1	B	480/504 (95%)	453 (94%)	24 (5%)	3 (1%)	21	27
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%)	48	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	428	GLY

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

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	417/436 (96%)	408 (98%)	9 (2%)	45	65
1	B	417/436 (96%)	403 (97%)	14 (3%)	32	49
1	C	418/436 (96%)	411 (98%)	7 (2%)	53	72
1	D	416/436 (95%)	404 (97%)	12 (3%)	37	55
1	E	417/436 (96%)	409 (98%)	8 (2%)	50	69
1	F	417/436 (96%)	406 (97%)	11 (3%)	40	59
All	All	2502/2616 (96%)	2441 (98%)	61 (2%)	43	62

All (61) 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	369	GLU
1	A	374	GLU
1	A	430	LYS
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

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Mol	Chain	Res	Type
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
1	C	75	ASN
1	C	292	LYS
1	C	354	VAL
1	C	363	LYS
1	C	369	GLU
1	C	382	MET
1	C	482	GLU
1	D	75	ASN
1	D	97	GLN
1	D	121	TYR
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	D	463	VAL
1	E	11	GLU
1	E	54	LEU
1	E	75	ASN
1	E	165	LYS
1	E	331	LEU
1	E	381	LYS
1	E	419	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	338	LYS
1	F	363	LYS
1	F	403	LYS

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Mol	Chain	Res	Type
1	F	415	GLU
1	F	430	LYS
1	F	448	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	C	102	ASN
1	C	158	HIS
1	C	388	ASN
1	D	19	HIS
1	D	64	ASN
1	D	323	ASN
1	D	365	HIS
1	D	452	ASN
1	E	98	GLN
1	E	146	ASN
1	E	158	HIS
1	E	313	GLN
1	E	469	HIS
1	F	181	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	485	-	7,7,7	0.50	0	9,9,9	1.24	1 (11%)
3	XYP	E	487	-	10,10,10	1.72	1 (10%)	14,14,14	1.43	2 (14%)
2	TRS	F	485	-	7,7,7	0.37	0	9,9,9	0.75	0
3	XYP	B	488	-	10,10,10	2.32	3 (30%)	14,14,14	2.98	8 (57%)
2	TRS	D	485	-	7,7,7	0.33	0	9,9,9	1.08	0
2	TRS	C	485	-	7,7,7	0.77	0	9,9,9	1.76	3 (33%)
3	XYP	B	489	-	10,10,10	2.46	5 (50%)	14,14,14	1.13	1 (7%)
3	XYP	D	490	-	10,10,10	1.86	4 (40%)	14,14,14	1.56	3 (21%)
2	TRS	D	486	-	7,7,7	0.51	0	9,9,9	1.36	1 (11%)
3	XYP	B	487	-	10,10,10	1.04	1 (10%)	14,14,14	0.39	0
3	XYP	D	488	-	10,10,10	2.37	3 (30%)	14,14,14	1.30	1 (7%)
2	TRS	C	486	-	7,7,7	0.69	0	9,9,9	1.23	0
3	XYP	C	487	-	10,10,10	1.37	1 (10%)	14,14,14	1.18	2 (14%)
3	XYP	A	489	-	10,10,10	2.71	4 (40%)	14,14,14	2.09	4 (28%)
3	XYP	D	489	-	10,10,10	2.07	4 (40%)	14,14,14	1.60	3 (21%)
3	XYP	D	487	-	10,10,10	2.10	4 (40%)	14,14,14	1.11	2 (14%)
2	TRS	B	486	-	7,7,7	0.29	0	9,9,9	1.71	3 (33%)
2	TRS	F	486	-	7,7,7	0.49	0	9,9,9	1.80	2 (22%)
2	TRS	A	485	-	7,7,7	0.36	0	9,9,9	0.69	0
3	XYP	A	488	-	10,10,10	4.12	5 (50%)	14,14,14	2.77	4 (28%)
2	TRS	A	486	-	7,7,7	0.36	0	9,9,9	1.56	2 (22%)
2	TRS	E	485	-	7,7,7	0.66	0	9,9,9	0.97	1 (11%)
3	XYP	F	487	-	10,10,10	1.79	2 (20%)	14,14,14	1.26	1 (7%)
3	XYP	C	488	-	10,10,10	2.33	3 (30%)	14,14,14	1.77	3 (21%)
2	TRS	E	486	-	7,7,7	0.34	0	9,9,9	1.13	0
3	XYP	E	488	-	10,10,10	2.41	4 (40%)	14,14,14	2.22	5 (35%)
3	XYP	A	487	-	10,10,10	1.21	0	14,14,14	1.26	2 (14%)

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	B	485	-	-	1/9/9/9	-
3	XYP	E	487	-	-	-	0/1/1/1
2	TRS	F	485	-	-	1/9/9/9	-
3	XYP	B	488	-	-	-	0/1/1/1
2	TRS	D	485	-	-	0/9/9/9	-
2	TRS	C	485	-	-	1/9/9/9	-
3	XYP	B	489	-	-	-	0/1/1/1
3	XYP	D	490	-	-	-	0/1/1/1
2	TRS	D	486	-	-	7/9/9/9	-
3	XYP	B	487	-	-	-	0/1/1/1
3	XYP	D	488	-	-	-	0/1/1/1
2	TRS	C	486	-	-	9/9/9/9	-
3	XYP	C	487	-	-	-	0/1/1/1
3	XYP	A	489	-	-	-	0/1/1/1
3	XYP	D	489	-	-	-	0/1/1/1
3	XYP	D	487	-	-	-	0/1/1/1
2	TRS	B	486	-	-	6/9/9/9	-
2	TRS	F	486	-	-	8/9/9/9	-
2	TRS	A	485	-	-	1/9/9/9	-
3	XYP	A	488	-	-	-	0/1/1/1
2	TRS	A	486	-	-	8/9/9/9	-
2	TRS	E	485	-	-	0/9/9/9	-
3	XYP	F	487	-	-	-	0/1/1/1
3	XYP	C	488	-	-	-	0/1/1/1
2	TRS	E	486	-	-	6/9/9/9	-
3	XYP	E	488	-	-	-	0/1/1/1
3	XYP	A	487	-	-	-	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	488	XYP	C4-C3	7.45	1.63	1.52
3	A	488	XYP	O4-C4	7.28	1.58	1.43
3	A	488	XYP	O5-C5	6.18	1.54	1.43
3	B	489	XYP	O5-C1	5.46	1.52	1.43
3	A	489	XYP	O5-C1	5.43	1.52	1.43
3	E	488	XYP	C4-C3	5.29	1.60	1.52
3	A	489	XYP	C4-C3	5.15	1.60	1.52
3	D	488	XYP	O5-C1	5.13	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	488	XYP	O5-C1	4.98	1.51	1.43
3	B	488	XYP	C4-C3	4.71	1.59	1.52
3	D	489	XYP	O5-C1	4.52	1.50	1.43
3	B	488	XYP	O2-C2	4.17	1.53	1.43
3	F	487	XYP	O5-C1	4.13	1.50	1.43
3	E	487	XYP	O5-C1	4.10	1.50	1.43
3	D	487	XYP	O5-C5	4.06	1.50	1.43
3	E	488	XYP	O5-C1	3.63	1.49	1.43
3	A	488	XYP	O5-C1	3.56	1.49	1.43
3	D	490	XYP	O1-C1	3.47	1.50	1.39
3	D	487	XYP	O5-C1	3.36	1.48	1.43
3	C	488	XYP	O5-C5	3.31	1.49	1.43
3	C	488	XYP	C4-C3	3.10	1.57	1.52
3	F	487	XYP	O5-C5	2.81	1.48	1.43
3	D	489	XYP	O5-C5	2.74	1.48	1.43
3	D	488	XYP	C4-C3	2.73	1.56	1.52
3	D	488	XYP	O1-C1	2.68	1.48	1.39
3	D	487	XYP	O1-C1	2.65	1.47	1.39
3	D	490	XYP	O3-C3	2.57	1.49	1.43
3	B	489	XYP	C4-C3	2.54	1.56	1.52
3	D	489	XYP	C4-C3	2.47	1.56	1.52
3	B	489	XYP	C1-C2	2.45	1.58	1.52
3	C	487	XYP	O5-C1	2.43	1.47	1.43
3	B	489	XYP	O1-C1	2.42	1.47	1.39
3	B	488	XYP	O5-C1	2.39	1.47	1.43
3	E	488	XYP	O5-C5	2.28	1.47	1.43
3	A	489	XYP	C1-C2	2.25	1.57	1.52
3	B	487	XYP	O5-C5	2.21	1.47	1.43
3	D	490	XYP	C1-C2	2.16	1.57	1.52
3	D	487	XYP	C4-C3	2.12	1.55	1.52
3	D	489	XYP	C1-C2	2.11	1.57	1.52
3	D	490	XYP	O5-C1	2.10	1.46	1.43
3	A	489	XYP	O1-C1	2.09	1.46	1.39
3	A	488	XYP	C3-C2	2.05	1.57	1.52
3	B	489	XYP	O5-C5	2.01	1.47	1.43
3	E	488	XYP	C5-C4	2.01	1.57	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	488	XYP	O5-C5-C4	6.96	127.39	110.79
3	B	488	XYP	C1-C2-C3	-5.35	99.45	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	488	XYP	O4-C4-C3	5.11	120.74	110.15
3	E	488	XYP	C1-C2-C3	-4.59	100.99	110.36
3	B	488	XYP	O1-C1-C2	4.59	122.29	108.98
3	B	488	XYP	O2-C2-C1	4.45	119.51	109.25
3	A	489	XYP	O3-C3-C4	4.12	118.45	110.05
3	B	488	XYP	O2-C2-C3	3.92	119.61	110.38
3	E	488	XYP	O3-C3-C4	3.87	117.94	110.05
3	A	489	XYP	O4-C4-C3	3.80	118.02	110.15
3	A	488	XYP	O3-C3-C4	3.48	117.17	110.05
2	C	485	TRS	C3-C-C2	-3.40	101.60	110.66
2	F	486	TRS	C3-C-C1	-3.37	101.67	110.66
3	D	489	XYP	C5-O5-C1	3.37	119.46	112.46
3	E	487	XYP	C5-C4-C3	3.36	114.54	109.64
3	D	490	XYP	O1-C1-C2	3.25	118.40	108.98
3	F	487	XYP	O1-C1-O5	3.20	118.10	109.91
3	B	488	XYP	O1-C1-O5	-3.15	101.83	109.91
2	A	486	TRS	O1-C1-C	-3.14	102.12	110.88
3	E	488	XYP	O4-C4-C3	3.12	116.61	110.15
2	F	486	TRS	O1-C1-C	3.11	119.54	110.88
3	C	488	XYP	C1-C2-C3	-3.09	104.05	110.36
3	B	488	XYP	O4-C4-C3	3.01	116.39	110.15
3	B	488	XYP	O3-C3-C4	2.97	116.11	110.05
3	D	490	XYP	O5-C5-C4	2.96	117.85	110.79
3	A	488	XYP	O1-C1-O5	2.96	117.48	109.91
3	D	489	XYP	O5-C5-C4	2.94	117.81	110.79
3	B	489	XYP	C5-C4-C3	2.90	113.87	109.64
3	C	488	XYP	O5-C5-C4	2.87	117.64	110.79
3	A	489	XYP	C5-O5-C1	2.77	118.21	112.46
3	C	488	XYP	C5-C4-C3	2.70	113.58	109.64
3	C	487	XYP	C5-O5-C1	2.68	118.02	112.46
2	B	486	TRS	O1-C1-C	-2.68	103.42	110.88
2	A	486	TRS	C2-C-C1	-2.65	103.59	110.66
3	A	489	XYP	C4-C3-C2	-2.53	106.42	110.86
2	B	486	TRS	C3-C-C1	-2.52	103.94	110.66
3	A	487	XYP	O4-C4-C3	-2.44	105.09	110.15
3	D	487	XYP	C5-O5-C1	2.40	117.44	112.46
2	D	486	TRS	C2-C-N	2.38	114.24	108.17
3	E	488	XYP	O2-C2-C1	2.35	114.68	109.25
2	C	485	TRS	C3-C-C1	2.33	116.87	110.66
3	A	487	XYP	C5-C4-C3	2.31	113.01	109.64
3	E	488	XYP	O2-C2-C3	2.25	115.68	110.38
2	C	485	TRS	C1-C-N	-2.23	102.48	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	487	XYP	O4-C4-C3	-2.22	105.56	110.15
3	D	488	XYP	C5-O5-C1	-2.14	108.01	112.46
2	E	485	TRS	C2-C-C1	-2.14	104.96	110.66
3	D	490	XYP	C5-C4-C3	2.13	112.75	109.64
3	D	489	XYP	O5-C1-C2	2.12	116.11	109.94
3	E	487	XYP	O1-C1-C2	2.10	115.09	108.98
2	B	485	TRS	C2-C-N	2.10	113.52	108.17
3	D	487	XYP	O1-C1-C2	2.07	114.99	108.98
2	B	486	TRS	C3-C-N	2.01	113.30	108.17
3	B	488	XYP	C4-C3-C2	-2.00	107.33	110.86

There are no chirality outliers.

All (48) 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
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

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

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	486	TRS	5	0
2	F	486	TRS	3	0
3	A	488	XYP	1	0
2	A	486	TRS	3	0
3	F	487	XYP	1	0
2	E	486	TRS	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	482/504 (95%)	-0.59	3 (0%) 85 86	21, 30, 50, 63	0
1	B	482/504 (95%)	-0.39	5 (1%) 79 80	23, 33, 52, 66	0
1	C	483/504 (95%)	-0.66	1 (0%) 91 91	21, 30, 48, 64	0
1	D	481/504 (95%)	-0.50	3 (0%) 85 86	22, 32, 50, 65	0
1	E	482/504 (95%)	-0.52	0 100 100	23, 32, 50, 64	0
1	F	482/504 (95%)	-0.55	3 (0%) 85 86	23, 32, 49, 64	0
All	All	2892/3024 (95%)	-0.53	15 (0%) 87 87	21, 32, 50, 66	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	483	LEU	4.6
1	B	382	MET	2.8
1	D	431	LYS	2.8
1	B	2	SER	2.6
1	F	382	MET	2.5
1	A	431	LYS	2.3
1	B	415	GLU	2.3
1	A	428	GLY	2.2
1	C	382	MET	2.2
1	A	382	MET	2.2
1	F	46	GLU	2.2
1	F	449	GLU	2.2
1	D	462	THR	2.2
1	B	431	LYS	2.1
1	D	415	GLU	2.1

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	XYP	E	488	10/10	0.71	0.22	64,75,77,79	0
3	XYP	A	488	10/10	0.76	0.17	44,55,58,59	0
3	XYP	C	488	10/10	0.82	0.18	68,73,76,77	0
3	XYP	D	488	10/10	0.83	0.15	51,61,67,69	0
3	XYP	B	488	10/10	0.83	0.15	43,56,59,64	0
3	XYP	B	489	10/10	0.85	0.15	62,68,70,71	0
3	XYP	A	489	10/10	0.86	0.16	52,59,60,63	0
2	TRS	C	486	8/8	0.89	0.18	45,50,51,52	0
3	XYP	D	489	10/10	0.90	0.12	55,60,62,65	0
3	XYP	D	490	10/10	0.91	0.11	54,60,61,63	0
3	XYP	C	487	10/10	0.92	0.10	44,48,49,52	0
2	TRS	B	486	8/8	0.92	0.11	42,43,45,46	0
2	TRS	E	486	8/8	0.92	0.12	47,48,51,51	0
2	TRS	D	486	8/8	0.93	0.10	34,39,42,43	0
2	TRS	F	486	8/8	0.93	0.13	51,53,54,55	0
2	TRS	A	486	8/8	0.94	0.10	41,45,46,48	0
3	XYP	D	487	10/10	0.94	0.08	43,47,49,51	0
3	XYP	F	487	10/10	0.94	0.09	49,50,53,53	0
3	XYP	A	487	10/10	0.95	0.07	38,40,41,41	0
3	XYP	E	487	10/10	0.95	0.07	43,46,49,49	0
3	XYP	B	487	10/10	0.96	0.07	44,47,48,48	0
2	TRS	E	485	8/8	0.97	0.06	31,32,33,34	0
2	TRS	A	485	8/8	0.97	0.06	28,30,32,32	0
2	TRS	C	485	8/8	0.97	0.06	22,25,27,28	0
2	TRS	B	485	8/8	0.98	0.05	27,29,29,31	0
2	TRS	F	485	8/8	0.98	0.05	32,32,33,33	0
2	TRS	D	485	8/8	0.98	0.05	28,30,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.