



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 04:36 AM EST

PDB ID : 5XIA  
Title : STRUCTURES OF D-XYLOSE ISOMERASE FROM ARTHROBACTER STRAIN B3728 CONTAINING THE INHIBITORS XYLITOL AND D-SORBITOL AT 2.5 ANGSTROMS AND 2.3 ANGSTROMS RESOLUTION, RESPECTIVELY  
Authors : Henrick, K.; Collyer, C.A.; Blow, D.M.  
Deposited on : unknown  
Resolution : 2.50 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](mailto: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.

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

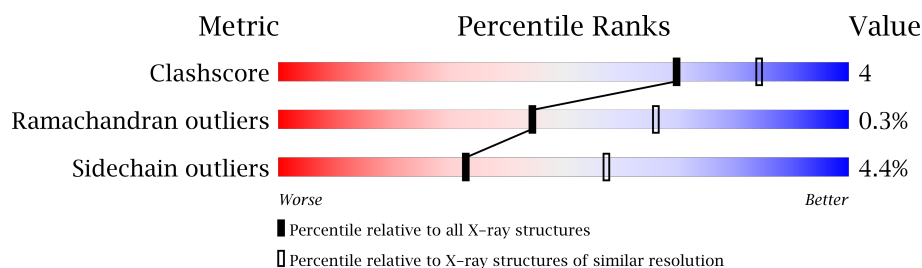
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	393	
1	B	393	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6651 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.

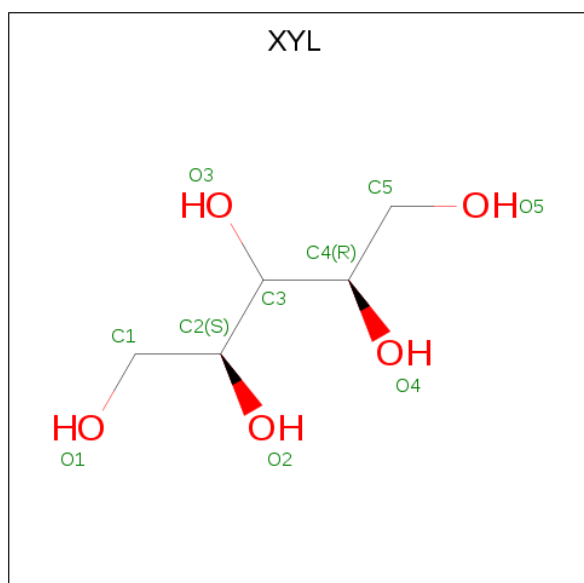
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3027	1919	520	579	9			
1	B	393	Total	C	N	O	S	0	0	0
			3027	1919	520	579	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ALA	LYS	CONFLICT	UNP P12070
A	64	ALA	GLU	CONFLICT	UNP P12070
A	79	ALA	LYS	CONFLICT	UNP P12070
B	31	ALA	LYS	CONFLICT	UNP P12070
B	64	ALA	GLU	CONFLICT	UNP P12070
B	79	ALA	LYS	CONFLICT	UNP P12070

- Molecule 2 is D-XYLITOL (three-letter code: XYL) (formula: C<sub>5</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

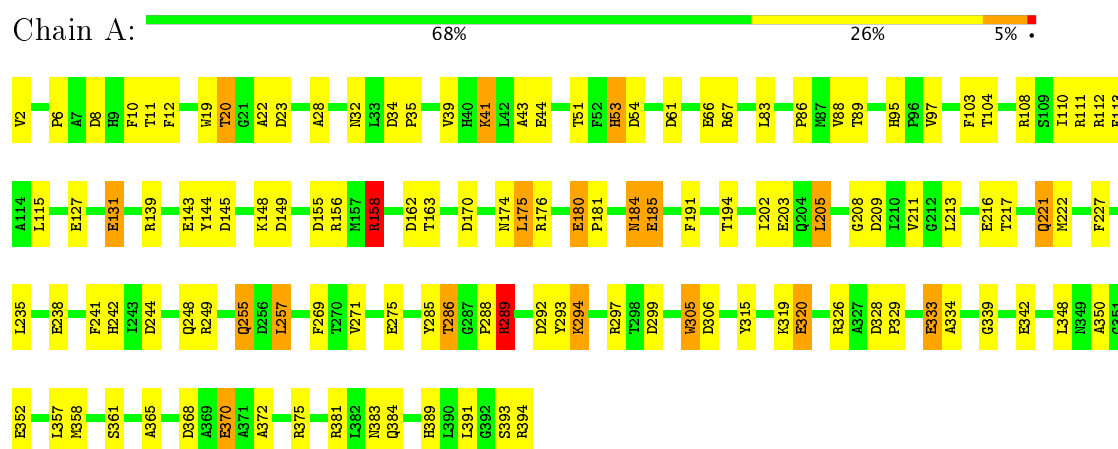
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	283	Total	O	0	0
			283	283		
4	B	292	Total	O	0	0
			292	292		

### 3 Residue-property plots

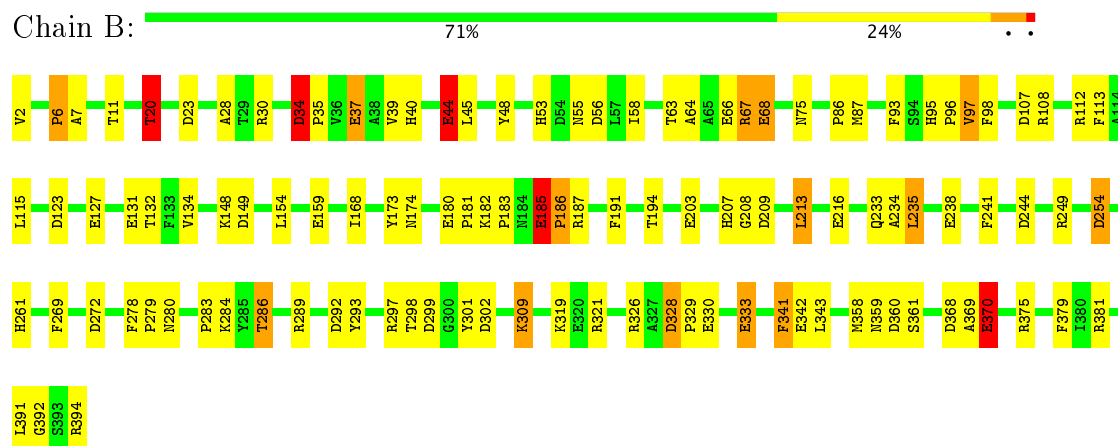
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

#### • Molecule 1: D-XYLOSE ISOMERASE



#### • Molecule 1: D-XYLOSE ISOMERASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.90 Å   105.90 Å   153.60 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.135 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6651	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

## 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: MG, XYL

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	1.25	4/3101 (0.1%)	2.36	154/4204 (3.7%)
1	B	1.25	6/3101 (0.2%)	2.12	109/4204 (2.6%)
All	All	1.25	10/6202 (0.2%)	2.24	263/8408 (3.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	ARG	CD-NE	-7.60	1.33	1.46
1	B	98	PHE	CE1-CZ	5.84	1.48	1.37
1	B	233	GLN	C-O	5.67	1.34	1.23
1	A	180	GLU	CD-OE1	-5.38	1.19	1.25
1	B	68	GLU	CD-OE2	5.36	1.31	1.25
1	A	339	GLY	C-O	5.28	1.32	1.23
1	B	392	GLY	N-CA	-5.27	1.38	1.46
1	B	297	ARG	CZ-NH2	5.13	1.39	1.33
1	A	216	GLU	CD-OE2	5.11	1.31	1.25
1	B	330	GLU	CD-OE1	-5.07	1.20	1.25

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	ARG	CD-NE-CZ	38.85	178.00	123.60
1	A	249	ARG	NE-CZ-NH1	23.73	132.16	120.30
1	A	112	ARG	NE-CZ-NH2	20.30	130.45	120.30
1	A	394	ARG	NE-CZ-NH2	-17.84	111.38	120.30
1	A	394	ARG	NE-CZ-NH1	16.31	128.45	120.30
1	B	375	ARG	NE-CZ-NH2	-15.91	112.34	120.30
1	B	381	ARG	NE-CZ-NH2	-14.92	112.84	120.30
1	B	30	ARG	NE-CZ-NH2	14.66	127.63	120.30
1	B	187	ARG	NE-CZ-NH1	14.43	127.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	PHE	CB-CG-CD1	14.35	130.84	120.80
1	B	123	ASP	CB-CG-OD1	13.98	130.88	118.30
1	A	394	ARG	CD-NE-CZ	13.34	142.27	123.60
1	A	139	ARG	NE-CZ-NH1	13.33	126.97	120.30
1	B	326	ARG	NE-CZ-NH2	-13.08	113.76	120.30
1	A	112	ARG	CD-NE-CZ	12.96	141.75	123.60
1	A	241	PHE	CB-CG-CD2	-12.87	111.79	120.80
1	B	394	ARG	NE-CZ-NH2	-12.80	113.90	120.30
1	B	238	GLU	CA-CB-CG	12.73	141.41	113.40
1	B	299	ASP	CB-CG-OD1	12.02	129.12	118.30
1	A	23	ASP	CB-CG-OD1	11.74	128.86	118.30
1	B	34	ASP	CB-CG-OD1	11.47	128.62	118.30
1	A	249	ARG	NE-CZ-NH2	-11.20	114.70	120.30
1	A	176	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	B	249	ARG	NE-CZ-NH1	10.81	125.70	120.30
1	A	111	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	A	289	ARG	NE-CZ-NH2	10.54	125.57	120.30
1	A	289	ARG	NE-CZ-NH1	-10.54	115.03	120.30
1	A	381	ARG	NE-CZ-NH1	10.45	125.52	120.30
1	A	381	ARG	NE-CZ-NH2	-10.40	115.10	120.30
1	B	381	ARG	CD-NE-CZ	10.37	138.12	123.60
1	A	149	ASP	CB-CG-OD1	10.25	127.53	118.30
1	B	30	ARG	NE-CZ-NH1	-9.97	115.31	120.30
1	B	187	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	A	145	ASP	CB-CG-OD2	-9.71	109.56	118.30
1	A	8	ASP	CB-CG-OD1	9.40	126.76	118.30
1	B	213	LEU	CA-CB-CG	9.39	136.89	115.30
1	A	43	ALA	CB-CA-C	9.32	124.09	110.10
1	A	299	ASP	CB-CG-OD1	9.27	126.64	118.30
1	A	145	ASP	CB-CG-OD1	9.12	126.50	118.30
1	B	326	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	A	156	ARG	NE-CZ-NH1	9.05	124.82	120.30
1	A	269	PHE	CB-CG-CD2	-9.02	114.49	120.80
1	A	342	GLU	OE1-CD-OE2	9.01	134.12	123.30
1	A	170	ASP	CB-CG-OD1	8.87	126.28	118.30
1	A	156	ARG	CD-NE-CZ	8.87	136.01	123.60
1	A	238	GLU	OE1-CD-OE2	8.78	133.84	123.30
1	B	112	ARG	CD-NE-CZ	8.62	135.68	123.60
1	A	326	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	112	ARG	NE-CZ-NH1	-8.51	116.04	120.30
1	A	127	GLU	CA-CB-CG	8.48	132.06	113.40
1	A	320	GLU	OE1-CD-OE2	-8.39	113.24	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ARG	CG-CD-NE	8.37	129.37	111.80
1	A	111	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	A	203	GLU	OE1-CD-OE2	-8.18	113.48	123.30
1	B	249	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	B	20	THR	N-CA-CB	-8.11	94.89	110.30
1	A	67	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	A	257	LEU	CA-CB-CG	8.09	133.90	115.30
1	A	289	ARG	CG-CD-NE	8.03	128.66	111.80
1	B	108	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	B	302	ASP	CB-CG-OD1	-7.93	111.16	118.30
1	B	360	ASP	CB-CG-OD1	7.82	125.34	118.30
1	B	391	LEU	C-N-CA	7.79	138.67	122.30
1	B	289	ARG	CD-NE-CZ	7.77	134.48	123.60
1	A	211	VAL	CA-CB-CG2	7.70	122.45	110.90
1	B	297	ARG	NE-CZ-NH2	7.69	124.14	120.30
1	A	216	GLU	OE1-CD-OE2	7.62	132.44	123.30
1	A	292	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	158	ARG	CD-NE-CZ	7.57	134.20	123.60
1	B	68	GLU	CB-CG-CD	7.57	134.63	114.20
1	B	241	PHE	CB-CG-CD2	-7.54	115.52	120.80
1	B	98	PHE	CB-CG-CD1	-7.54	115.52	120.80
1	B	48	TYR	CB-CG-CD2	-7.51	116.49	121.00
1	B	44	GLU	CG-CD-OE2	-7.50	103.29	118.30
1	A	158	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	108	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	A	144	TYR	CB-CG-CD1	7.43	125.46	121.00
1	B	23	ASP	CB-CA-C	7.40	125.21	110.40
1	A	393	SER	C-N-CA	7.39	140.17	121.70
1	A	194	THR	CA-CB-CG2	7.35	122.70	112.40
1	A	203	GLU	CG-CD-OE1	7.33	132.97	118.30
1	B	368	ASP	CB-CG-OD2	7.27	124.85	118.30
1	B	123	ASP	OD1-CG-OD2	-7.24	109.54	123.30
1	B	20	THR	CA-CB-CG2	7.23	122.52	112.40
1	A	320	GLU	CA-CB-CG	7.20	129.24	113.40
1	A	108	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	A	67	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	272	ASP	CB-CG-OD1	7.17	124.75	118.30
1	B	319	LYS	CB-CG-CD	7.09	130.04	111.60
1	A	175	LEU	CA-CB-CG	7.07	131.56	115.30
1	A	139	ARG	NH1-CZ-NH2	-7.07	111.63	119.40
1	B	293	TYR	CB-CG-CD1	-7.05	116.77	121.00
1	A	285	TYR	CB-CG-CD2	-7.00	116.80	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ASN	N-CA-CB	6.97	123.15	110.60
1	B	7	ALA	N-CA-CB	-6.94	100.39	110.10
1	A	23	ASP	CB-CG-OD2	-6.91	112.09	118.30
1	A	320	GLU	CG-CD-OE1	6.87	132.03	118.30
1	B	44	GLU	CG-CD-OE1	6.86	132.03	118.30
1	A	12	PHE	CB-CG-CD1	-6.83	116.02	120.80
1	A	44	GLU	CA-CB-CG	6.81	128.39	113.40
1	A	235	LEU	CB-CA-C	6.79	123.09	110.20
1	B	286	THR	N-CA-CB	-6.78	97.42	110.30
1	A	155	ASP	CB-CG-OD2	6.75	124.37	118.30
1	A	6	PRO	C-N-CA	6.75	138.57	121.70
1	A	149	ASP	N-CA-CB	6.71	122.69	110.60
1	A	391	LEU	C-N-CA	6.71	136.39	122.30
1	B	23	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	44	GLU	N-CA-CB	6.68	122.62	110.60
1	B	6	PRO	O-C-N	-6.67	112.02	122.70
1	A	352	GLU	CG-CD-OE1	6.65	131.61	118.30
1	A	326	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	A	352	GLU	OE1-CD-OE2	-6.63	115.34	123.30
1	A	293	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	B	301	TYR	CB-CG-CD2	-6.61	117.03	121.00
1	B	394	ARG	NH1-CZ-NH2	6.59	126.66	119.40
1	B	358	MET	C-N-CA	6.55	138.07	121.70
1	A	185	GLU	CG-CD-OE1	6.54	131.37	118.30
1	B	381	ARG	NH1-CZ-NH2	6.52	126.58	119.40
1	A	357	LEU	CB-CG-CD2	-6.50	99.95	111.00
1	B	96	PRO	O-C-N	-6.50	112.30	122.70
1	B	174	ASN	CB-CG-OD1	6.48	134.56	121.60
1	A	368	ASP	CB-CG-OD1	6.45	124.10	118.30
1	A	139	ARG	CD-NE-CZ	6.38	132.53	123.60
1	A	176	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	286	THR	N-CA-CB	-6.35	98.23	110.30
1	B	127	GLU	CA-CB-CG	6.35	127.36	113.40
1	B	37	GLU	CB-CG-CD	6.31	131.24	114.20
1	A	144	TYR	CB-CG-CD2	-6.29	117.23	121.00
1	B	292	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	350	ALA	CB-CA-C	6.25	119.47	110.10
1	A	286	THR	CA-CB-OG1	-6.24	95.90	109.00
1	B	194	THR	CA-CB-CG2	6.20	121.08	112.40
1	A	115	LEU	CB-CA-C	6.20	121.97	110.20
1	A	43	ALA	O-C-N	-6.19	112.80	122.70
1	B	113	PHE	CB-CG-CD1	-6.18	116.47	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	VAL	CA-CB-CG1	6.18	120.17	110.90
1	A	244	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	372	ALA	O-C-N	-6.16	112.85	122.70
1	B	23	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	185	GLU	OE1-CD-OE2	-6.13	115.94	123.30
1	A	113	PHE	CB-CG-CD1	-6.13	116.51	120.80
1	A	127	GLU	CG-CD-OE2	-6.13	106.05	118.30
1	A	51	THR	CA-CB-CG2	6.11	120.96	112.40
1	A	297	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	B	131	GLU	CB-CG-CD	6.07	130.58	114.20
1	B	23	ASP	OD1-CG-OD2	-6.04	111.83	123.30
1	A	113	PHE	CB-CG-CD2	6.03	125.02	120.80
1	B	333	GLU	CA-CB-CG	6.02	126.65	113.40
1	A	235	LEU	O-C-N	-6.02	113.06	122.70
1	B	203	GLU	CG-CD-OE1	6.02	130.34	118.30
1	A	249	ARG	CD-NE-CZ	5.95	131.93	123.60
1	B	342	GLU	CG-CD-OE2	-5.95	106.41	118.30
1	A	131	GLU	CB-CG-CD	5.93	130.22	114.20
1	A	175	LEU	O-C-N	5.91	132.16	122.70
1	A	12	PHE	CB-CG-CD2	5.86	124.91	120.80
1	A	103	PHE	CB-CG-CD1	5.85	124.90	120.80
1	B	343	LEU	C-N-CA	5.84	134.56	122.30
1	A	34	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	131	GLU	OE1-CD-OE2	-5.83	116.30	123.30
1	B	298	THR	O-C-N	-5.83	113.37	122.70
1	B	113	PHE	CB-CG-CD2	5.82	124.87	120.80
1	B	134	VAL	CA-CB-CG1	5.82	119.62	110.90
1	A	156	ARG	CA-CB-CG	5.81	126.18	113.40
1	A	54	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	19	TRP	N-CA-CB	5.77	120.99	110.60
1	B	159	GLU	CG-CD-OE2	-5.76	106.78	118.30
1	B	209	ASP	CB-CG-OD1	5.76	123.48	118.30
1	B	369	ALA	CB-CA-C	5.76	118.73	110.10
1	A	249	ARG	NH1-CZ-NH2	-5.75	113.07	119.40
1	A	389	HIS	N-CA-CB	5.75	120.95	110.60
1	B	238	GLU	CB-CG-CD	5.75	129.72	114.20
1	A	22	ALA	N-CA-CB	-5.75	102.05	110.10
1	A	269	PHE	CZ-CE2-CD2	-5.73	113.23	120.10
1	A	163	THR	CA-CB-CG2	5.71	120.40	112.40
1	B	216	GLU	CG-CD-OE1	5.71	129.72	118.30
1	A	88	VAL	CA-CB-CG2	5.70	119.45	110.90
1	B	391	LEU	CA-CB-CG	5.66	128.32	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	PHE	CA-C-O	-5.65	108.23	120.10
1	A	180	GLU	CG-CD-OE1	5.65	129.60	118.30
1	B	299	ASP	OD1-CG-OD2	-5.64	112.59	123.30
1	B	107	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	127	GLU	OE1-CD-OE2	5.63	130.05	123.30
1	A	205	LEU	CA-CB-CG	5.60	128.19	115.30
1	B	154	LEU	CB-CA-C	5.59	120.82	110.20
1	B	379	PHE	O-C-N	-5.56	113.80	122.70
1	A	110	ILE	O-C-N	-5.55	113.82	122.70
1	A	149	ASP	N-CA-C	-5.54	96.03	111.00
1	A	170	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	B	6	PRO	C-N-CA	5.54	135.54	121.70
1	B	370	GLU	CG-CD-OE2	-5.52	107.25	118.30
1	B	20	THR	CB-CA-C	5.51	126.48	111.60
1	A	269	PHE	CB-CG-CD1	5.50	124.65	120.80
1	B	2	VAL	C-N-CA	5.50	135.44	121.70
1	A	66	GLU	CG-CD-OE1	5.47	129.23	118.30
1	B	269	PHE	CD1-CE1-CZ	-5.46	113.55	120.10
1	A	292	ASP	OD1-CG-OD2	-5.46	112.93	123.30
1	B	298	THR	C-N-CA	5.45	135.32	121.70
1	A	61	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	315	TYR	CB-CG-CD1	5.42	124.25	121.00
1	B	56	ASP	N-CA-CB	5.41	120.33	110.60
1	A	53	HIS	N-CA-CB	5.40	120.31	110.60
1	B	328	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	112	ARG	NH1-CZ-NH2	-5.38	113.49	119.40
1	B	97	VAL	CG1-CB-CG2	-5.37	102.31	110.90
1	A	6	PRO	O-C-N	-5.36	114.12	122.70
1	B	53	HIS	N-CA-CB	5.34	120.22	110.60
1	A	294	LYS	CD-CE-NZ	5.33	123.96	111.70
1	A	222	MET	C-N-CA	5.31	134.99	121.70
1	B	64	ALA	N-CA-CB	5.30	117.52	110.10
1	B	333	GLU	CG-CD-OE2	-5.29	107.71	118.30
1	A	375	ARG	CD-NE-CZ	-5.29	116.19	123.60
1	B	342	GLU	CB-CG-CD	5.29	128.48	114.20
1	B	98	PHE	CB-CG-CD2	5.28	124.50	120.80
1	A	333	GLU	CA-CB-CG	5.27	125.00	113.40
1	B	341	PHE	CB-CG-CD1	-5.27	117.11	120.80
1	B	359	ASN	CB-CA-C	-5.26	99.87	110.40
1	A	184	ASN	C-N-CA	5.25	134.83	121.70
1	A	32	ASN	CA-CB-CG	-5.25	101.85	113.40
1	A	365	ALA	CA-C-N	5.25	126.70	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	306	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	115	LEU	CB-CA-C	5.24	120.15	110.20
1	A	143	GLU	CA-C-O	5.23	131.09	120.10
1	A	158	ARG	CB-CG-CD	5.22	125.17	111.60
1	A	352	GLU	CA-CB-CG	5.22	124.88	113.40
1	A	162	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	143	GLU	OE1-CD-OE2	-5.21	117.05	123.30
1	B	234	ALA	CB-CA-C	5.20	117.90	110.10
1	A	10	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	B	375	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	320	GLU	CB-CG-CD	5.18	128.20	114.20
1	A	334	ALA	CB-CA-C	5.18	117.87	110.10
1	B	53	HIS	CA-CB-CG	5.18	122.41	113.60
1	A	127	GLU	O-C-N	-5.18	114.42	122.70
1	A	108	ARG	NH1-CZ-NH2	-5.17	113.72	119.40
1	A	19	TRP	C-N-CA	5.16	134.60	121.70
1	B	286	THR	OG1-CB-CG2	5.15	121.85	110.00
1	B	186	PRO	N-CA-C	5.15	125.49	112.10
1	A	358	MET	C-N-CA	5.15	134.57	121.70
1	A	209	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	348	LEU	CA-CB-CG	5.14	127.12	115.30
1	B	6	PRO	CA-C-N	5.13	128.48	117.20
1	A	156	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	284	LYS	CA-CB-CG	5.12	124.67	113.40
1	A	208	GLY	O-C-N	-5.12	114.51	122.70
1	A	271	VAL	O-C-N	-5.12	114.51	122.70
1	A	305	TRP	CB-CA-C	5.12	120.64	110.40
1	B	44	GLU	CA-C-N	5.12	128.46	117.20
1	B	131	GLU	CG-CD-OE1	5.11	128.53	118.30
1	A	208	GLY	C-N-CA	5.11	134.48	121.70
1	B	207	HIS	O-C-N	-5.10	114.52	123.20
1	B	244	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	370	GLU	CG-CD-OE2	-5.09	108.12	118.30
1	A	370	GLU	OE1-CD-OE2	5.09	129.40	123.30
1	A	104	THR	CA-CB-CG2	5.07	119.49	112.40
1	A	297	ARG	C-N-CA	5.07	134.36	121.70
1	A	255	GLN	N-CA-CB	-5.05	101.52	110.60
1	B	254	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	B	216	GLU	CG-CD-OE2	-5.04	108.23	118.30
1	A	342	GLU	CB-CA-C	-5.01	100.38	110.40
1	A	383	ASN	O-C-N	-5.01	114.68	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	GLN	O-C-N	-5.01	114.69	122.70
1	B	321	ARG	CA-CB-CG	-5.00	102.39	113.40

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	3027	0	2890	25	0
1	B	3027	0	2891	26	0
2	A	10	0	11	0	0
2	B	10	0	10	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	283	0	0	3	0
4	B	292	0	0	3	0
All	All	6651	0	5802	50	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 4.

All (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLU:HG3	1:A:319:LYS:HG3	1.67	0.76
1:B:95:HIS:HD2	1:B:97:VAL:H	1.34	0.72
1:B:235:LEU:HD22	1:B:283:PRO:HB2	1.76	0.68
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.64	0.62
1:A:294:LYS:HE2	4:A:641:HOH:O	2.02	0.58
1:A:95:HIS:HD2	1:A:97:VAL:H	1.51	0.57
1:B:45:LEU:HD22	1:B:309:LYS:HD3	1.87	0.57
1:B:208:GLY:HA3	4:B:599:HOH:O	2.09	0.53
1:B:55:ASN:HA	1:B:58:ILE:O	2.08	0.53
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ARG:HG3	1:A:205:LEU:HD23	1.91	0.51
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.92	0.51
1:A:20:THR:HG23	1:A:28:ALA:HB1	1.95	0.49
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.49	0.48
1:A:370:GLU:HG2	4:A:644:HOH:O	2.13	0.48
1:A:41:LYS:HG2	1:A:305:TRP:CE2	2.49	0.47
1:B:370:GLU:HG2	4:B:678:HOH:O	2.14	0.47
1:B:328:ASP:HA	1:B:329:PRO:HD3	1.69	0.46
1:B:168:ILE:HG23	1:B:173:TYR:HB2	1.96	0.46
1:B:180:GLU:HA	1:B:181:PRO:HD3	1.81	0.45
1:A:158:ARG:HB3	4:A:465:HOH:O	2.16	0.45
1:B:34:ASP:HA	1:B:35:PRO:HD3	1.77	0.45
1:A:328:ASP:HA	1:A:329:PRO:HD3	1.77	0.45
1:B:35:PRO:O	1:B:39:VAL:HG23	2.17	0.45
1:B:20:THR:HG23	1:B:28:ALA:CB	2.47	0.44
1:A:217:THR:HA	1:A:227:PHE:CD2	2.52	0.44
1:A:255:GLN:HB3	1:A:257:LEU:HG	1.97	0.44
1:A:35:PRO:O	1:A:39:VAL:HG23	2.17	0.44
1:B:45:LEU:HD22	1:B:309:LYS:CD	2.47	0.44
1:A:20:THR:HG23	1:A:28:ALA:CB	2.48	0.44
1:B:11:THR:HG21	1:B:86:PRO:HG2	2.00	0.44
1:A:242:HIS:CD2	1:A:288:PRO:HG2	2.54	0.43
1:B:75:ASN:ND2	4:B:665:HOH:O	2.51	0.43
1:A:202:ILE:O	1:A:205:LEU:HB2	2.18	0.43
1:B:148:LYS:HG3	1:B:191:PHE:HZ	1.83	0.43
1:B:280:ASN:OD1	1:B:341:PHE:HA	2.19	0.43
1:B:278:PHE:HA	1:B:279:PRO:HD3	1.92	0.42
1:B:63:THR:HG23	1:B:66:GLU:OE1	2.20	0.42
1:B:185:GLU:HA	1:B:186:PRO:HA	1.84	0.42
1:A:95:HIS:CD2	1:A:97:VAL:H	2.34	0.42
1:A:384:GLN:NE2	1:B:261:HIS:NE2	2.67	0.42
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.85	0.41
1:B:40:HIS:O	1:B:44:GLU:HG3	2.21	0.41
1:A:289:ARG:HD2	1:A:289:ARG:N	2.35	0.41
1:B:182:LYS:HA	1:B:183:PRO:HD3	1.88	0.41
1:A:131:GLU:O	1:A:175:LEU:HA	2.21	0.41
1:B:95:HIS:CD2	1:B:97:VAL:H	2.25	0.40
1:A:180:GLU:HA	1:A:181:PRO:HD3	1.82	0.40
1:A:2:VAL:O	1:A:2:VAL:HG23	2.21	0.40
1:B:87:MET:HA	1:B:132:THR:O	2.21	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	391/393 (100%)	377 (96%)	13 (3%)	1 (0%)	44	66
1	B	391/393 (100%)	375 (96%)	15 (4%)	1 (0%)	44	66
All	All	782/786 (100%)	752 (96%)	28 (4%)	2 (0%)	44	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU
1	B	185	GLU

### 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	305/306 (100%)	295 (97%)	10 (3%)	43	70
1	B	305/306 (100%)	288 (94%)	17 (6%)	25	45
All	All	610/612 (100%)	583 (96%)	27 (4%)	33	57

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	41	LYS
1	A	158	ARG
1	A	184	ASN

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Mol	Chain	Res	Type
1	A	213	LEU
1	A	286	THR
1	A	289	ARG
1	A	320	GLU
1	A	333	GLU
1	A	361	SER
1	B	6	PRO
1	B	20	THR
1	B	34	ASP
1	B	37	GLU
1	B	44	GLU
1	B	67	ARG
1	B	68	GLU
1	B	149	ASP
1	B	185	GLU
1	B	213	LEU
1	B	235	LEU
1	B	254	ASP
1	B	286	THR
1	B	309	LYS
1	B	333	GLU
1	B	361	SER
1	B	370	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	95	HIS
1	A	184	ASN
1	A	384	GLN
1	B	75	ASN
1	B	76	GLN
1	B	95	HIS
1	B	120	HIS
1	B	384	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	XYL	A	400	3	9,9,9	0.82	0	11,11,11	1.75	3 (27%)
2	XYL	B	400	3	9,9,9	0.97	1 (11%)	11,11,11	1.31	1 (9%)

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	XYL	A	400	3	-	0/12/12/12	0/0/0/0
2	XYL	B	400	3	-	0/12/12/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	XYL	O3-C3	2.44	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	XYL	O5-C5-C4	-2.97	104.56	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	XYL	O2-C2-C1	-2.17	104.19	109.21
2	A	400	XYL	O4-C4-C5	2.68	115.41	109.21
2	A	400	XYL	C5-C4-C3	3.77	120.82	112.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.