



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 09:33 PM BST

PDB ID : 1XLG  
Title : MECHANISM FOR ALDOSE-KETOSE INTERCONVERSION BY D-XYLOSE ISOMERASE INVOLVING RING OPENING FOLLOWED BY A 1,2-HYDRIDE SHIFT  
Authors : Collyer, C.A.; Henrick, K.; Blow, D.M.  
Deposited on : 1991-10-09  
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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

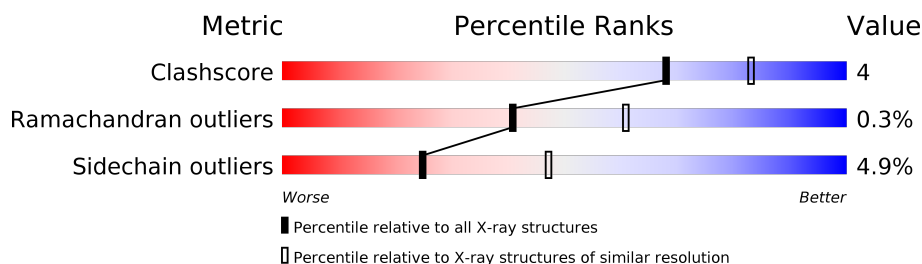
# 1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	394	
1	B	394	

## 2 Entry composition [i](#)

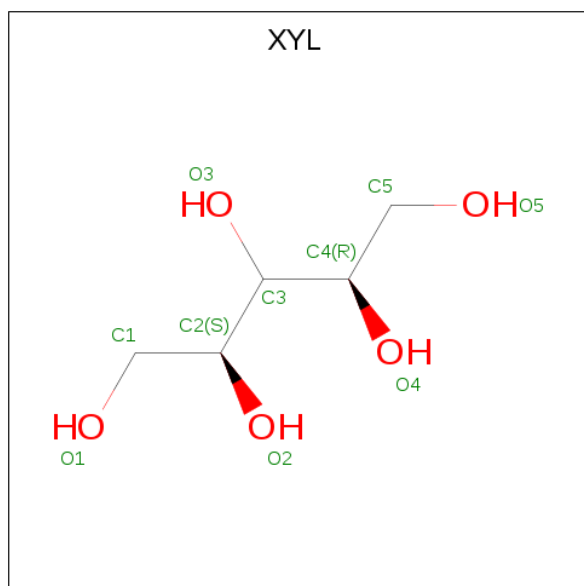
There are 5 unique types of molecules in this entry. The entry contains 6614 atoms, of which 0 are hydrogens and 0 are deuteriums.

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			

- Molecule 2 is 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 1 1	0	0
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is ALUMINUM ION (three-letter code: AL) (formula: Al).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Al 1 1	0	0
4	A	1	Total Al 1 1	0	0

- Molecule 5 is water.

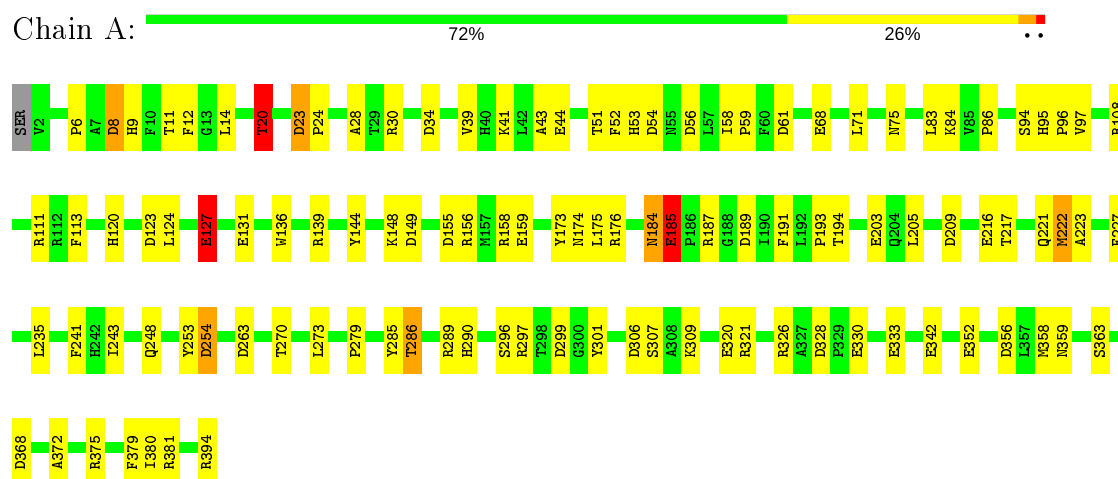
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	266	Total O 266 266	0	0
5	B	270	Total O 270 270	0	0

### 3 Residue-property plots

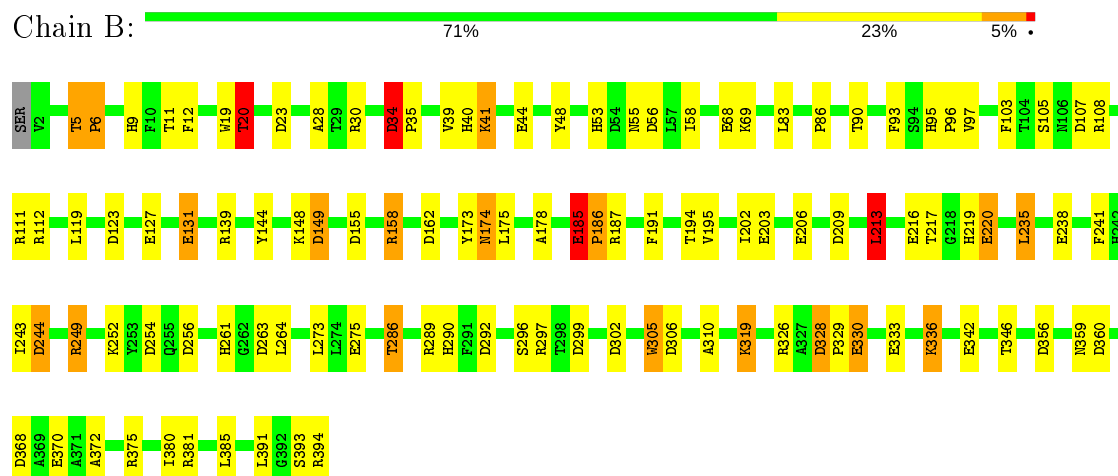
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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, $\alpha$ , $\beta$ , $\gamma$	105.80 Å   105.80 Å   153.20 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.158 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6614	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, XYL, AL

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	1.07	1/3101 (0.0%)	2.04	101/4204 (2.4%)
1	B	1.11	1/3101 (0.0%)	2.06	104/4204 (2.5%)
All	All	1.09	2/6202 (0.0%)	2.05	205/8408 (2.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	GLU	CD-OE2	6.61	1.32	1.25
1	B	105	SER	C-O	5.50	1.33	1.23

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	ARG	NE-CZ-NH2	-22.57	109.02	120.30
1	A	375	ARG	NE-CZ-NH2	-17.26	111.67	120.30
1	B	187	ARG	NE-CZ-NH1	16.78	128.69	120.30
1	A	156	ARG	NE-CZ-NH1	14.63	127.61	120.30
1	A	156	ARG	NE-CZ-NH2	-14.06	113.27	120.30
1	B	158	ARG	NE-CZ-NH2	-13.73	113.44	120.30
1	B	111	ARG	NE-CZ-NH1	13.53	127.06	120.30
1	A	187	ARG	NE-CZ-NH2	-13.00	113.80	120.30
1	B	381	ARG	NE-CZ-NH2	-12.09	114.26	120.30
1	A	187	ARG	NE-CZ-NH1	12.04	126.32	120.30
1	A	131	GLU	CB-CG-CD	11.98	146.56	114.20
1	B	34	ASP	CB-CG-OD2	11.87	128.98	118.30
1	A	139	ARG	NE-CZ-NH1	11.09	125.84	120.30
1	B	30	ARG	NE-CZ-NH1	11.04	125.82	120.30
1	B	297	ARG	NE-CZ-NH2	11.03	125.81	120.30
1	B	299	ASP	CB-CG-OD1	10.86	128.07	118.30
1	A	253	TYR	CB-CG-CD1	10.85	127.51	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	ASP	CB-CG-OD2	10.70	127.92	118.30
1	B	158	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	A	30	ARG	NE-CZ-NH2	-9.79	115.41	120.30
1	A	285	TYR	CB-CG-CD2	-9.62	115.22	121.00
1	B	249	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	B	360	ASP	CB-CG-OD2	9.26	126.64	118.30
1	B	394	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	A	111	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	A	144	TYR	CB-CG-CD2	8.85	126.31	121.00
1	A	289	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	B	206	GLU	CA-CB-CG	8.76	132.68	113.40
1	B	326	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	B	209	ASP	CB-CG-OD2	8.67	126.11	118.30
1	B	368	ASP	CB-CG-OD2	8.66	126.10	118.30
1	A	375	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	B	330	GLU	CA-CB-CG	8.54	132.18	113.40
1	B	306	ASP	CB-CG-OD2	8.53	125.98	118.30
1	A	285	TYR	CB-CG-CD1	8.49	126.09	121.00
1	A	144	TYR	CB-CG-CD1	-8.48	115.91	121.00
1	A	253	TYR	CB-CG-CD2	-8.47	115.92	121.00
1	B	292	ASP	CB-CG-OD1	8.31	125.78	118.30
1	A	6	PRO	C-N-CA	8.27	142.37	121.70
1	B	112	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	B	173	TYR	CB-CG-CD1	8.12	125.88	121.00
1	A	342	GLU	OE1-CD-OE2	8.09	133.01	123.30
1	A	326	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	B	20	THR	N-CA-CB	-7.97	95.15	110.30
1	A	108	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	B	9	HIS	CA-CB-CG	7.92	127.07	113.60
1	A	176	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	358	MET	C-N-CA	7.86	141.36	121.70
1	A	30	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	111	ARG	CA-CB-CG	7.76	130.48	113.40
1	B	263	ASP	CB-CG-OD2	7.76	125.28	118.30
1	A	185	GLU	OE1-CD-OE2	7.72	132.56	123.30
1	B	289	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	A	113	PHE	CB-CG-CD2	-7.66	115.44	120.80
1	A	149	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	342	GLU	CG-CD-OE2	-7.61	103.07	118.30
1	B	131	GLU	OE1-CD-OE2	-7.55	114.24	123.30
1	A	34	ASP	CB-CG-OD2	7.36	124.92	118.30
1	B	5	THR	CA-CB-CG2	7.31	122.64	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	299	ASP	CB-CG-OD1	7.26	124.83	118.30
1	B	20	THR	CA-CB-CG2	7.25	122.55	112.40
1	B	336	LYS	CB-CA-C	7.20	124.81	110.40
1	A	320	GLU	CA-CB-CG	7.15	129.13	113.40
1	A	241	PHE	CB-CG-CD1	7.13	125.80	120.80
1	A	301	TYR	CB-CG-CD2	-7.09	116.75	121.00
1	A	379	PHE	CB-CG-CD2	-7.08	115.84	120.80
1	A	6	PRO	O-C-N	-7.03	111.46	122.70
1	A	194	THR	CA-CB-CG2	6.97	122.16	112.40
1	A	185	GLU	CG-CD-OE1	-6.93	104.43	118.30
1	A	84	LYS	C-N-CA	6.92	139.01	121.70
1	A	68	GLU	OE1-CD-OE2	6.91	131.60	123.30
1	A	56	ASP	CB-CG-OD2	6.90	124.51	118.30
1	B	155	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	B	194	THR	CA-CB-CG2	6.88	122.03	112.40
1	A	320	GLU	CG-CD-OE2	6.84	131.97	118.30
1	B	249	ARG	CA-C-N	6.82	129.85	116.20
1	B	149	ASP	CB-CG-OD1	6.81	124.43	118.30
1	B	342	GLU	CG-CD-OE2	-6.79	104.72	118.30
1	B	23	ASP	CB-CA-C	6.77	123.94	110.40
1	B	238	GLU	CG-CD-OE1	6.71	131.71	118.30
1	A	54	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	8	ASP	CB-CG-OD2	6.67	124.31	118.30
1	B	328	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	52	PHE	CB-CG-CD2	-6.56	116.21	120.80
1	B	173	TYR	CB-CG-CD2	-6.56	117.06	121.00
1	B	178	ALA	CB-CA-C	6.55	119.92	110.10
1	B	203	GLU	CG-CD-OE2	6.53	131.36	118.30
1	A	289	ARG	CA-CB-CG	6.52	127.74	113.40
1	A	333	GLU	CA-CB-CG	6.52	127.74	113.40
1	B	30	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	270	THR	CA-CB-CG2	6.37	121.32	112.40
1	B	375	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	127	GLU	CA-CB-CG	6.33	127.33	113.40
1	A	149	ASP	N-CA-C	-6.33	93.91	111.00
1	B	139	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	B	256	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	174	ASN	C-N-CA	6.27	137.38	121.70
1	A	356	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	220	GLU	OE1-CD-OE2	6.14	130.67	123.30
1	A	189	ASP	CB-CG-OD1	6.13	123.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ASP	CB-CG-OD1	6.13	123.82	118.30
1	B	394	ARG	NH1-CZ-NH2	6.12	126.14	119.40
1	A	372	ALA	O-C-N	-6.11	112.93	122.70
1	A	51	THR	CA-CB-CG2	6.10	120.94	112.40
1	A	263	ASP	CB-CG-OD1	6.08	123.77	118.30
1	B	286	THR	CA-CB-CG2	6.06	120.89	112.40
1	A	320	GLU	OE1-CD-OE2	-6.04	116.06	123.30
1	B	241	PHE	CB-CG-CD2	-6.04	116.58	120.80
1	A	155	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	B	149	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	B	203	GLU	OE1-CD-OE2	-5.99	116.11	123.30
1	B	107	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	B	203	GLU	O-C-N	-5.95	113.18	122.70
1	B	108	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	A	111	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	372	ALA	CB-CA-C	5.87	118.90	110.10
1	B	123	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	219	HIS	CB-CG-ND1	-5.87	108.53	123.20
1	A	352	GLU	OE1-CD-OE2	-5.86	116.27	123.30
1	B	330	GLU	CG-CD-OE1	-5.86	106.59	118.30
1	B	96	PRO	CA-C-N	5.84	130.06	117.20
1	A	297	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	286	THR	N-CA-CB	-5.84	99.21	110.30
1	A	203	GLU	CG-CD-OE2	5.81	129.92	118.30
1	B	175	LEU	CA-CB-CG	5.81	128.66	115.30
1	B	149	ASP	N-CA-C	-5.79	95.36	111.00
1	A	175	LEU	CB-CA-C	-5.79	99.20	110.20
1	B	12	PHE	N-CA-CB	5.79	121.02	110.60
1	A	39	VAL	CA-CB-CG2	5.77	119.55	110.90
1	B	56	ASP	N-CA-CB	5.77	120.98	110.60
1	A	216	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	A	352	GLU	N-CA-CB	5.75	120.95	110.60
1	A	83	LEU	CA-CB-CG	5.74	128.50	115.30
1	B	302	ASP	CB-CG-OD1	5.74	123.47	118.30
1	B	305	TRP	CB-CA-C	5.71	121.82	110.40
1	A	379	PHE	CB-CG-CD1	5.70	124.79	120.80
1	B	299	ASP	OD1-CG-OD2	-5.70	112.47	123.30
1	A	175	LEU	CA-CB-CG	5.65	128.30	115.30
1	A	328	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	279	PRO	O-C-N	-5.63	113.69	122.70
1	B	360	ASP	OD1-CG-OD2	-5.63	112.61	123.30
1	A	381	ARG	NE-CZ-NH1	5.62	123.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	TYR	CB-CG-CD2	5.60	124.36	121.00
1	B	93	PHE	CB-CG-CD1	5.59	124.71	120.80
1	A	394	ARG	CD-NE-CZ	5.58	131.42	123.60
1	B	174	ASN	OD1-CG-ND2	5.58	134.74	121.90
1	B	48	TYR	CB-CG-CD1	-5.56	117.66	121.00
1	B	53	HIS	N-CA-CB	5.56	120.61	110.60
1	B	186	PRO	N-CA-C	5.55	126.52	112.10
1	B	261	HIS	C-N-CA	5.55	133.95	122.30
1	A	286	THR	CA-CB-OG1	-5.54	97.37	109.00
1	B	333	GLU	CG-CD-OE1	5.53	129.36	118.30
1	A	297	ARG	O-C-N	-5.49	113.92	122.70
1	A	127	GLU	CG-CD-OE2	-5.48	107.34	118.30
1	A	44	GLU	CA-CB-CG	5.48	125.45	113.40
1	B	68	GLU	OE1-CD-OE2	-5.48	116.73	123.30
1	A	306	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	12	PHE	CB-CG-CD1	-5.46	116.97	120.80
1	A	139	ARG	NH1-CZ-NH2	-5.44	113.42	119.40
1	B	319	LYS	C-N-CA	5.44	135.29	121.70
1	B	302	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	A	352	GLU	N-CA-C	-5.43	96.34	111.00
1	A	173	TYR	CB-CG-CD1	5.42	124.25	121.00
1	A	53	HIS	N-CA-CB	5.39	120.30	110.60
1	A	368	ASP	OD1-CG-OD2	-5.39	113.06	123.30
1	B	385	LEU	CB-CA-C	5.38	120.43	110.20
1	B	356	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	310	ALA	CB-CA-C	5.37	118.16	110.10
1	B	264	LEU	CB-CG-CD2	-5.34	101.91	111.00
1	B	19	TRP	N-CA-CB	5.34	120.22	110.60
1	A	20	THR	N-CA-CB	-5.33	100.18	110.30
1	B	391	LEU	C-N-CA	5.33	133.48	122.30
1	B	203	GLU	C-N-CA	5.32	135.01	121.70
1	B	254	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	12	PHE	C-N-CA	-5.32	111.14	122.30
1	A	96	PRO	O-C-N	-5.31	114.20	122.70
1	B	162	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	136	TRP	N-CA-CB	5.28	120.11	110.60
1	B	103	PHE	CB-CG-CD1	5.28	124.50	120.80
1	B	44	GLU	CG-CD-OE1	-5.28	107.75	118.30
1	B	310	ALA	O-C-N	-5.26	114.28	122.70
1	A	321	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	238	GLU	OE1-CD-OE2	-5.23	117.03	123.30
1	A	159	GLU	CA-CB-CG	5.22	124.89	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	GLU	CG-CD-OE2	5.21	128.71	118.30
1	B	217	THR	C-N-CA	5.17	133.17	122.30
1	B	119	LEU	CB-CA-C	5.16	120.00	110.20
1	B	368	ASP	OD1-CG-OD2	-5.15	113.51	123.30
1	B	40	HIS	CA-CB-CG	-5.15	104.85	113.60
1	A	61	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	254	ASP	N-CA-CB	5.13	119.83	110.60
1	B	372	ALA	O-C-N	-5.13	114.49	122.70
1	B	6	PRO	C-N-CA	5.12	134.51	121.70
1	A	223	ALA	C-N-CA	5.11	133.03	122.30
1	B	346	THR	CA-CB-OG1	-5.10	98.30	109.00
1	B	213	LEU	CA-CB-CG	5.09	127.02	115.30
1	B	23	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	222	MET	C-N-CA	5.09	134.43	121.70
1	A	193	PRO	N-CA-C	5.09	125.33	112.10
1	A	14	LEU	O-C-N	-5.05	114.61	122.70
1	A	56	ASP	C-N-CA	5.05	134.34	121.70
1	A	356	ASP	CB-CG-OD1	-5.03	113.78	118.30
1	A	43	ALA	O-C-N	-5.02	114.66	122.70
1	B	244	ASP	CB-CG-OD1	5.01	122.81	118.30

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	2879	24	0
1	B	3027	0	2882	25	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	1	0	0	0	0
4	B	1	0	0	0	0
5	A	266	0	0	2	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	270	0	0	1	0
All	All	6614	0	5782	45	2

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 (45) 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:B:275:GLU:HG3	1:B:319:LYS:HG3	1.63	0.81
1:A:95:HIS:HD2	1:A:97:VAL:H	1.35	0.75
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.73	0.70
1:B:95:HIS:HD2	1:B:97:VAL:H	1.40	0.67
1:A:235:LEU:HD12	1:A:273:LEU:HD21	1.77	0.66
1:B:235:LEU:HD12	1:B:273:LEU:HD21	1.79	0.65
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.79	0.63
1:A:158:ARG:HG3	1:A:205:LEU:HD23	1.80	0.63
1:B:148:LYS:HG3	1:B:191:PHE:HZ	1.70	0.56
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.88	0.56
1:A:184:ASN:HD22	1:A:185:GLU:HB2	1.72	0.54
1:A:95:HIS:CD2	1:A:97:VAL:H	2.23	0.54
1:A:296:SER:H	1:B:380:ILE:HD11	1.74	0.53
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.73	0.52
1:A:124:LEU:HA	1:A:127:GLU:HG3	1.93	0.51
1:B:55:ASN:HA	1:B:58:ILE:O	2.13	0.48
1:B:158:ARG:HD2	5:B:737(B):HOH:O	2.12	0.48
1:B:202:ILE:HD11	1:B:213:LEU:HD23	1.96	0.48
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.79	0.47
1:A:380:ILE:HD11	1:B:296:SER:HB2	1.96	0.47
1:B:249:ARG:O	1:B:252:LYS:HE3	2.13	0.47
1:A:20:THR:HG23	1:A:28:ALA:CB	2.44	0.47
1:A:75:ASN:ND2	5:A:568(A):HOH:O	2.48	0.46
1:A:296:SER:N	1:B:380:ILE:HD11	2.30	0.46
1:B:20:THR:HG23	1:B:28:ALA:CB	2.45	0.46
1:A:307:SER:HB3	1:B:380:ILE:HG21	1.98	0.45
1:A:222:MET:SD	1:A:254:ASP:HB3	2.56	0.45
1:B:243:ILE:O	1:B:290:HIS:HB3	2.17	0.45
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.99	0.44
1:B:41:LYS:HG2	1:B:305:TRP:CD2	2.52	0.44
1:B:41:LYS:HG2	1:B:305:TRP:CE2	2.52	0.43
1:B:34:ASP:HA	1:B:35:PRO:HD3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ILE:HD11	1:A:71:LEU:HD21	2.01	0.43
1:B:328:ASP:HA	1:B:329:PRO:HD3	1.80	0.42
1:B:95:HIS:CD2	1:B:97:VAL:H	2.29	0.42
1:A:120:HIS:O	1:A:123:ASP:HB2	2.20	0.42
1:A:217:THR:HA	1:A:227:PHE:CD1	2.55	0.41
1:A:8:ASP:O	1:A:9:HIS:HB2	2.20	0.41
1:A:59:PRO:HG2	5:A:564(A):HOH:O	2.19	0.41
1:A:23:ASP:HB2	1:A:24:PRO:CD	2.50	0.41
1:A:243:ILE:O	1:A:290:HIS:HB3	2.21	0.41
1:B:195:VAL:HG23	1:B:220:GLU:CD	2.41	0.41
1:B:216:GLU:HA	1:B:244:ASP:O	2.21	0.41
1:A:20:THR:HG23	1:A:28:ALA:HB1	2.02	0.40
1:B:185:GLU:HA	1:B:186:PRO:HA	1.78	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:477(A):HOH:O	5:A:630(A):HOH:O[4_555]	2.10	0.10
5:A:473(A):HOH:O	5:A:596(A):HOH:O[4_555]	2.11	0.09

## 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	391/394 (99%)	376 (96%)	14 (4%)	1 (0%)	41	61
1	B	391/394 (99%)	376 (96%)	14 (4%)	1 (0%)	41	61
All	All	782/788 (99%)	752 (96%)	28 (4%)	2 (0%)	41	61

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	305/310 (98%)	294 (96%)	11 (4%)	35	61
1	B	305/310 (98%)	286 (94%)	19 (6%)	18	35
All	All	610/620 (98%)	580 (95%)	30 (5%)	25	47

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	41	LYS
1	A	94	SER
1	A	127	GLU
1	A	184	ASN
1	A	185	GLU
1	A	286	THR
1	A	309	LYS
1	A	330	GLU
1	A	359	ASN
1	A	363	SER
1	B	5	THR
1	B	6	PRO
1	B	20	THR
1	B	34	ASP
1	B	41	LYS
1	B	69	LYS
1	B	90	THR
1	B	131	GLU
1	B	149	ASP
1	B	174	ASN
1	B	185	GLU

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Mol	Chain	Res	Type
1	B	213	LEU
1	B	235	LEU
1	B	286	THR
1	B	330	GLU
1	B	336	LYS
1	B	359	ASN
1	B	370	GLU
1	B	393	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	75	ASN
1	A	95	HIS
1	A	184	ASN
1	A	221	GLN
1	A	384	GLN
1	B	9	HIS
1	B	95	HIS
1	B	184	ASN
1	B	204	GLN
1	B	359	ASN
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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 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	B	400	3,4	9,9,9	0.82	1 (11%)	11,11,11	1.74	2 (18%)
2	XYL	A	400	3,4	9,9,9	0.86	0	11,11,11	1.82	4 (36%)

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	B	400	3,4	-	0/12/12/12	-
2	XYL	A	400	3,4	-	0/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	XYL	C4-C3	-2.18	1.49	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	XYL	C4-C3-C2	3.51	120.67	113.36
2	A	400	XYL	C4-C3-C2	3.19	120.01	113.36
2	A	400	XYL	O2-C2-C3	3.12	116.69	109.10
2	B	400	XYL	O1-C1-C2	2.76	117.10	111.07
2	A	400	XYL	O2-C2-C1	-2.37	103.59	109.14
2	A	400	XYL	C1-C2-C3	-2.18	107.69	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.