



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:30 PM GMT

PDB ID : 1XLJ
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

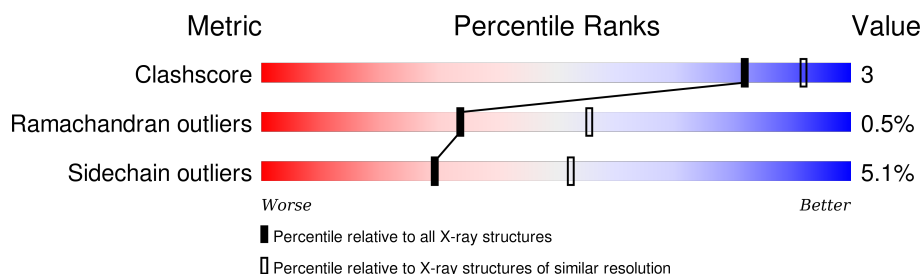
1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 ≥ 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	394	 71% 24% . .
1	B	394	 73% 24% . .

2 Entry composition [i](#)

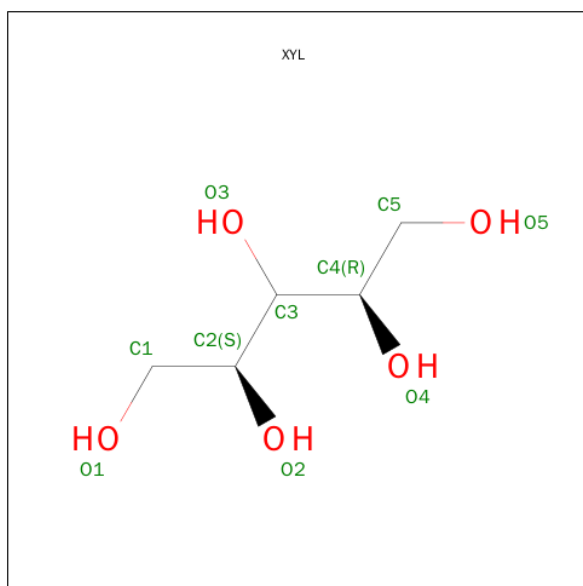
There are 4 unique types of molecules in this entry. The entry contains 6590 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-XYLITOL (three-letter code: XYL) (formula: $C_5H_{12}O_5$).



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 MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is water.

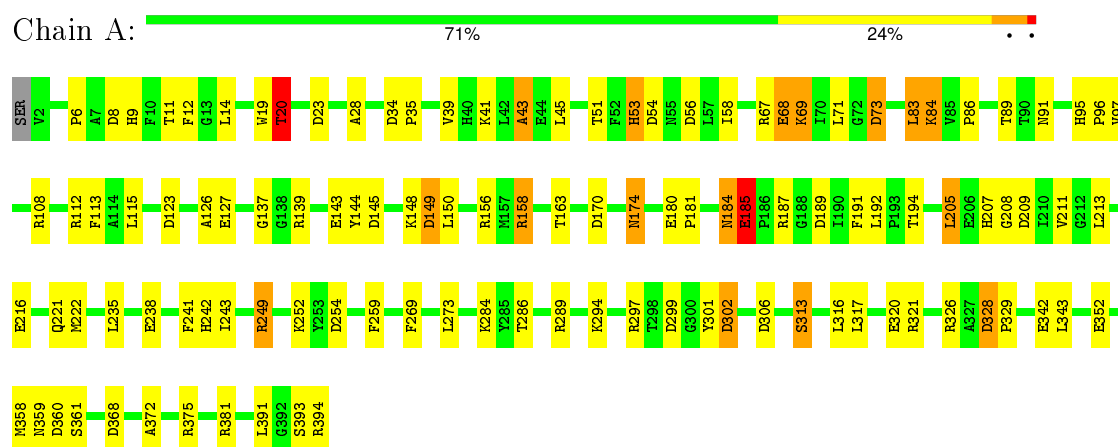
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	256	Total 256	O 256	0	0
4	B	258	Total 258	O 258	0	0

3 Residue-property plots

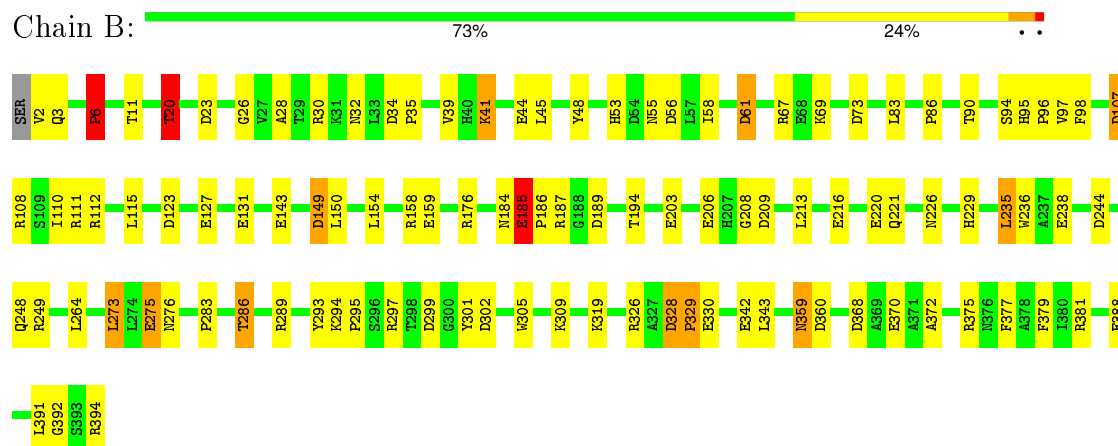
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.90 Å 105.90 Å 153.60 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}	0.156 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6590	wwPDB-VP
Average B, all atoms (Å ²)	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: MN, 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	1.11	1/3101 (0.0%)	2.09	124/4204 (2.9%)
1	B	1.14	1/3101 (0.0%)	2.05	98/4204 (2.3%)
All	All	1.13	2/6202 (0.0%)	2.07	222/8408 (2.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	SER	CB-OG	-6.12	1.34	1.42
1	B	238	GLU	CB-CG	5.16	1.61	1.52

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ARG	NE-CZ-NH1	16.27	128.44	120.30
1	A	23	ASP	CB-CG-OD1	16.08	132.77	118.30
1	B	187	ARG	NE-CZ-NH2	-15.55	112.52	120.30
1	B	381	ARG	NE-CZ-NH2	-15.31	112.64	120.30
1	B	108	ARG	NE-CZ-NH2	-14.00	113.30	120.30
1	A	249	ARG	NE-CZ-NH1	13.94	127.27	120.30
1	B	112	ARG	CD-NE-CZ	13.72	142.81	123.60
1	B	123	ASP	CB-CG-OD2	13.20	130.18	118.30
1	B	30	ARG	NE-CZ-NH1	12.57	126.58	120.30
1	B	249	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	B	108	ARG	NE-CZ-NH1	11.68	126.14	120.30
1	B	187	ARG	NE-CZ-NH1	11.65	126.13	120.30
1	A	269	PHE	CB-CG-CD1	-11.64	112.65	120.80
1	B	299	ASP	CB-CG-OD1	11.55	128.69	118.30
1	B	394	ARG	NE-CZ-NH2	-11.34	114.63	120.30
1	A	139	ARG	NE-CZ-NH2	11.19	125.90	120.30
1	B	30	ARG	NE-CZ-NH2	-11.02	114.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ASP	CB-CG-OD2	-11.00	108.40	118.30
1	B	375	ARG	NE-CZ-NH2	-10.83	114.88	120.30
1	A	241	PHE	CB-CG-CD1	10.80	128.36	120.80
1	B	297	ARG	NE-CZ-NH2	10.64	125.62	120.30
1	B	293	TYR	CB-CG-CD2	-10.64	114.62	121.00
1	A	68	GLU	OE1-CD-OE2	10.14	135.46	123.30
1	A	394	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	A	149	ASP	CB-CG-OD1	9.88	127.19	118.30
1	A	23	ASP	CB-CG-OD2	-9.80	109.48	118.30
1	B	359	ASN	CA-CB-CG	9.57	134.46	113.40
1	B	209	ASP	CB-CG-OD2	9.47	126.83	118.30
1	B	213	LEU	CA-CB-CG	9.42	136.97	115.30
1	A	108	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	A	156	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	A	299	ASP	CB-CG-OD1	9.19	126.57	118.30
1	A	342	GLU	CA-CB-CG	9.10	133.41	113.40
1	A	123	ASP	CB-CG-OD1	9.08	126.47	118.30
1	A	394	ARG	CD-NE-CZ	8.88	136.04	123.60
1	A	6	PRO	C-N-CA	8.86	143.84	121.70
1	A	51	THR	CA-CB-CG2	8.77	124.68	112.40
1	B	20	THR	N-CA-CB	-8.60	93.96	110.30
1	B	328	ASP	CB-CG-OD1	8.51	125.96	118.30
1	A	73	ASP	CB-CG-OD2	-8.40	110.74	118.30
1	B	23	ASP	CB-CA-C	8.39	127.17	110.40
1	A	297	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	B	372	ALA	CB-CA-C	8.14	122.32	110.10
1	A	368	ASP	CB-CG-OD2	8.12	125.61	118.30
1	B	368	ASP	CB-CG-OD1	8.11	125.60	118.30
1	A	12	PHE	CB-CG-CD1	-8.04	115.18	120.80
1	B	127	GLU	CA-CB-CG	7.89	130.75	113.40
1	A	194	THR	CA-CB-CG2	7.85	123.38	112.40
1	A	269	PHE	CB-CG-CD2	7.76	126.23	120.80
1	A	34	ASP	CB-CG-OD1	7.75	125.28	118.30
1	A	6	PRO	O-C-N	-7.74	110.31	122.70
1	B	372	ALA	O-C-N	-7.68	110.42	122.70
1	A	145	ASP	CB-CG-OD1	7.66	125.20	118.30
1	A	342	GLU	OE1-CD-OE2	7.66	132.49	123.30
1	B	149	ASP	CB-CG-OD1	7.64	125.17	118.30
1	A	241	PHE	CB-CG-CD2	-7.59	115.49	120.80
1	A	249	ARG	CD-NE-CZ	7.58	134.22	123.60
1	B	379	PHE	CB-CG-CD1	7.57	126.10	120.80
1	B	2	VAL	C-N-CA	7.57	140.61	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	ARG	NE-CZ-NH1	-7.54	116.53	120.30
1	A	8	ASP	CB-CG-OD2	7.49	125.04	118.30
1	A	163	THR	CA-CB-CG2	7.41	122.77	112.40
1	A	375	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	B	244	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	320	GLU	CA-CB-CG	7.28	129.41	113.40
1	A	328	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	216	GLU	OE1-CD-OE2	7.25	132.00	123.30
1	B	53	HIS	N-CA-CB	7.24	123.64	110.60
1	A	289	ARG	CD-NE-CZ	7.24	133.73	123.60
1	A	67	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	B	203	GLU	CG-CD-OE2	7.19	132.69	118.30
1	A	393	SER	C-N-CA	7.19	139.67	121.70
1	B	20	THR	CA-CB-CG2	7.17	122.43	112.40
1	B	342	GLU	CG-CD-OE2	-7.16	103.98	118.30
1	A	149	ASP	N-CA-CB	7.13	123.44	110.60
1	B	302	ASP	CB-CG-OD2	-7.12	111.90	118.30
1	A	123	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	A	20	THR	CA-CB-CG2	7.07	122.30	112.40
1	A	174	ASN	N-CA-CB	7.07	123.32	110.60
1	A	301	TYR	CB-CG-CD2	-7.04	116.77	121.00
1	A	73	ASP	CB-CG-OD1	7.04	124.64	118.30
1	A	343	LEU	C-N-CA	7.00	137.00	122.30
1	A	358	MET	C-N-CA	6.98	139.16	121.70
1	A	368	ASP	OD1-CG-OD2	-6.98	110.03	123.30
1	B	123	ASP	OD1-CG-OD2	-6.96	110.07	123.30
1	A	108	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	289	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	111	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	381	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	326	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	206	GLU	CA-CB-CG	6.87	128.50	113.40
1	B	34	ASP	CB-CG-OD2	6.85	124.47	118.30
1	A	342	GLU	N-CA-CB	6.79	122.82	110.60
1	A	368	ASP	CB-CG-OD1	6.72	124.35	118.30
1	B	273	LEU	CA-CB-CG	6.68	130.67	115.30
1	B	330	GLU	OE1-CD-OE2	6.63	131.25	123.30
1	B	32	ASN	CA-CB-CG	-6.62	98.83	113.40
1	A	12	PHE	CB-CG-CD2	6.52	125.36	120.80
1	A	238	GLU	OE1-CD-OE2	6.51	131.11	123.30
1	B	149	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	A	320	GLU	CG-CD-OE2	6.46	131.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	ALA	O-C-N	-6.43	112.41	122.70
1	A	375	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	189	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	A	127	GLU	CA-CB-CG	6.38	127.43	113.40
1	A	306	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	273	LEU	CA-CB-CG	6.36	129.92	115.30
1	A	316	LEU	CB-CA-C	6.35	122.26	110.20
1	A	301	TYR	CB-CG-CD1	6.33	124.80	121.00
1	A	189	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	159	GLU	CA-CB-CG	6.29	127.23	113.40
1	B	189	ASP	CB-CG-OD2	6.28	123.95	118.30
1	B	203	GLU	OE1-CD-OE2	-6.25	115.80	123.30
1	A	187	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	6	PRO	CA-C-N	6.22	130.89	117.20
1	B	238	GLU	CG-CD-OE2	6.17	130.64	118.30
1	A	112	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	326	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	B	286	THR	N-CA-CB	-6.13	98.64	110.30
1	B	194	THR	CA-CB-CG2	6.12	120.97	112.40
1	B	391	LEU	C-N-CA	6.10	135.12	122.30
1	B	342	GLU	OE1-CD-OE2	6.10	130.62	123.30
1	A	360	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	249	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	A	139	ARG	NH1-CZ-NH2	-6.06	112.73	119.40
1	B	108	ARG	CD-NE-CZ	6.04	132.06	123.60
1	B	275	GLU	C-N-CA	6.03	136.78	121.70
1	A	112	ARG	CD-NE-CZ	6.02	132.03	123.60
1	B	127	GLU	CG-CD-OE2	6.02	130.34	118.30
1	A	149	ASP	N-CA-C	-6.01	94.76	111.00
1	A	19	TRP	C-N-CA	6.01	136.73	121.70
1	B	360	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	302	ASP	CB-CG-OD1	5.98	123.68	118.30
1	B	176	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	54	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	170	ASP	CB-CG-OD1	5.95	123.66	118.30
1	B	379	PHE	CA-CB-CG	5.95	128.17	113.90
1	A	113	PHE	CB-CG-CD2	-5.93	116.64	120.80
1	B	343	LEU	C-N-CA	5.93	134.76	122.30
1	A	222	MET	C-N-CA	5.88	136.41	121.70
1	B	189	ASP	CB-CG-OD1	-5.88	113.01	118.30
1	A	8	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	A	170	ASP	CB-CG-OD2	-5.85	113.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ALA	CB-CA-C	5.81	118.81	110.10
1	B	379	PHE	CB-CA-C	5.79	121.99	110.40
1	A	53	HIS	N-CA-CB	5.79	121.02	110.60
1	B	273	LEU	CB-CG-CD1	5.78	120.83	111.00
1	A	96	PRO	O-C-N	-5.77	113.47	122.70
1	B	220	GLU	OE1-CD-OE2	5.75	130.20	123.30
1	B	236	TRP	CA-CB-CG	5.75	124.62	113.70
1	B	44	GLU	N-CA-CB	5.74	120.93	110.60
1	A	221	GLN	C-N-CA	5.73	136.02	121.70
1	B	264	LEU	CB-CG-CD2	-5.72	101.27	111.00
1	A	158	ARG	CD-NE-CZ	5.70	131.58	123.60
1	A	235	LEU	O-C-N	-5.69	113.59	122.70
1	B	56	ASP	N-CA-CB	5.68	120.82	110.60
1	A	56	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	B	297	ARG	NH1-CZ-NH2	-5.65	113.18	119.40
1	A	352	GLU	CG-CD-OE2	5.63	129.57	118.30
1	A	381	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	149	ASP	OD1-CG-OD2	-5.63	112.61	123.30
1	A	14	LEU	C-N-CA	5.62	135.74	121.70
1	A	43	ALA	O-C-N	-5.61	113.73	122.70
1	A	143	GLU	OE1-CD-OE2	-5.61	116.57	123.30
1	A	302	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	A	53	HIS	CB-CA-C	-5.57	99.26	110.40
1	A	205	LEU	CA-CB-CG	5.57	128.10	115.30
1	B	20	THR	CB-CA-C	5.54	126.57	111.60
1	B	391	LEU	O-C-N	-5.52	113.81	123.20
1	A	313	SER	N-CA-CB	-5.52	102.22	110.50
1	B	107	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	249	ARG	NH1-CZ-NH2	-5.49	113.36	119.40
1	A	137	GLY	C-N-CA	5.49	133.83	122.30
1	A	211	VAL	CA-CB-CG2	5.49	119.13	110.90
1	B	96	PRO	O-C-N	-5.45	113.98	122.70
1	A	381	ARG	CD-NE-CZ	5.45	131.23	123.60
1	B	115	LEU	CB-CA-C	5.42	120.50	110.20
1	B	73	ASP	CA-CB-CG	5.42	125.32	113.40
1	A	83	LEU	CB-CA-C	5.40	120.46	110.20
1	A	342	GLU	CB-CA-C	-5.38	99.64	110.40
1	A	144	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	A	14	LEU	O-C-N	-5.37	114.11	122.70
1	B	377	PHE	CB-CG-CD2	-5.36	117.05	120.80
1	A	207	HIS	O-C-N	-5.35	114.11	123.20
1	B	143	GLU	OE1-CD-OE2	-5.35	116.88	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	379	PHE	CB-CG-CD2	-5.34	117.06	120.80
1	B	149	ASP	N-CA-C	-5.34	96.58	111.00
1	A	91	ASN	CB-CG-OD1	5.32	132.24	121.60
1	B	61	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	23	ASP	CB-CA-C	5.31	121.01	110.40
1	A	84	LYS	CB-CA-C	5.31	121.01	110.40
1	A	43	ALA	CB-CA-C	5.29	118.04	110.10
1	B	293	TYR	CB-CG-CD1	5.28	124.17	121.00
1	B	176	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	67	ARG	CG-CD-NE	5.27	122.87	111.80
1	A	391	LEU	C-N-CA	5.25	133.34	122.30
1	B	26	GLY	N-CA-C	5.24	126.20	113.10
1	A	192	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	259	PHE	C-N-CA	5.21	133.25	122.30
1	B	301	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	B	131	GLU	CG-CD-OE1	5.18	128.67	118.30
1	B	216	GLU	CG-CD-OE1	5.17	128.63	118.30
1	A	208	GLY	O-C-N	-5.15	114.46	122.70
1	A	156	ARG	CA-CB-CG	5.14	124.72	113.40
1	A	20	THR	N-CA-CB	-5.14	100.53	110.30
1	B	150	LEU	CB-CA-C	5.14	119.97	110.20
1	A	289	ARG	N-CA-C	-5.11	97.20	111.00
1	A	221	GLN	N-CA-CB	-5.10	101.42	110.60
1	A	209	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	34	ASP	OD1-CG-OD2	-5.08	113.64	123.30
1	A	221	GLN	O-C-N	-5.08	114.58	122.70
1	A	243	ILE	O-C-N	5.06	130.80	122.70
1	B	370	GLU	CG-CD-OE1	-5.06	108.17	118.30
1	B	388	GLU	O-C-N	-5.05	114.61	122.70
1	B	98	PHE	CB-CG-CD2	-5.05	117.27	120.80
1	A	127	GLU	N-CA-CB	5.04	119.66	110.60
1	B	392	GLY	C-N-CA	5.02	134.26	121.70
1	A	242	HIS	CB-CA-C	5.02	120.45	110.40
1	B	48	TYR	N-CA-CB	-5.02	101.56	110.60
1	A	115	LEU	CB-CA-C	5.01	119.73	110.20
1	B	44	GLU	CG-CD-OE1	-5.01	108.27	118.30
1	B	154	LEU	CB-CA-C	5.00	119.71	110.20

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	2880	19	1
1	B	3027	0	2881	19	1
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	256	0	0	2	1
4	B	258	0	0	1	0
All	All	6590	0	5782	38	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 3.

All (38) 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:95:HIS:HD2	1:A:97:VAL:H	1.34	0.75
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.71	0.71
1:B:95:HIS:HD2	1:B:97:VAL:H	1.39	0.70
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.63	0.64
1:A:58:ILE:HD11	1:A:71:LEU:HD21	1.84	0.60
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.85	0.57
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.87	0.57
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.88	0.54
1:B:235:LEU:HD22	1:B:283:PRO:HB2	1.90	0.54
1:A:69:LYS:HE2	1:A:73:ASP:OD2	2.09	0.53
1:A:84:LYS:HD2	4:A:423(A):HOH:O	2.10	0.50
1:A:20:THR:HG23	1:A:28:ALA:HB1	1.94	0.50
1:A:158:ARG:HG3	1:A:205:LEU:HD23	1.95	0.49
1:A:43:ALA:HB2	1:A:83:LEU:HD13	1.95	0.49
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.49	0.48
1:B:107:ASP:HB3	1:B:110:ILE:HD12	1.96	0.47
1:B:20:THR:HG23	1:B:28:ALA:CB	2.45	0.47
1:B:45:LEU:HD22	1:B:309:LYS:HG3	1.96	0.47
1:B:328:ASP:HA	1:B:329:PRO:HD3	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:PRO:O	1:B:39:VAL:HG23	2.15	0.46
1:A:184:ASN:HD22	1:A:185:GLU:HB2	1.81	0.45
1:A:41:LYS:O	1:A:45:LEU:HG	2.16	0.45
1:A:317:LEU:O	1:A:321:ARG:HD2	2.17	0.45
1:A:328:ASP:HA	1:A:329:PRO:HD3	1.82	0.45
1:B:221:GLN:HE21	1:B:248:GLN:HB3	1.81	0.45
1:B:226:ASN:HB3	1:B:229:HIS:HB2	2.00	0.44
1:B:41:LYS:HG2	1:B:305:TRP:CD2	2.52	0.44
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.99	0.43
1:A:294:LYS:NZ	4:A:464(A):HOH:O	2.46	0.43
1:B:309:LYS:HE2	1:B:309:LYS:HB3	1.62	0.42
1:B:55:ASN:HA	1:B:58:ILE:O	2.20	0.41
1:A:95:HIS:CD2	1:A:97:VAL:H	2.24	0.41
1:B:185:GLU:HA	1:B:186:PRO:HA	1.87	0.41
1:B:294:LYS:HA	1:B:295:PRO:HD3	1.94	0.41
1:A:249:ARG:O	1:A:252:LYS:HE3	2.21	0.41
1:A:180:GLU:HA	1:A:181:PRO:HD3	1.74	0.40
1:A:35:PRO:O	1:A:39:VAL:HG23	2.21	0.40
1:B:208:GLY:HA3	4:B:590(B):HOH:O	2.20	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)
1:A:69:LYS:NZ	1:B:276:ASN:O[6_665]	2.04	0.16
4:A:461(A):HOH:O	4:A:584(A):HOH:O[4_555]	2.17	0.03

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%)	374 (96%)	16 (4%)	1 (0%)	46 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	391/394 (99%)	375 (96%)	13 (3%)	3 (1%)	24	41
All	All	782/788 (99%)	749 (96%)	29 (4%)	4 (0%)	34	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU
1	B	185	GLU
1	B	3	GLN
1	B	6	PRO

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%)	289 (95%)	16 (5%)	29	51
1	B	305/310 (98%)	290 (95%)	15 (5%)	31	55
All	All	610/620 (98%)	579 (95%)	31 (5%)	29	52

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	20	THR
1	A	68	GLU
1	A	69	LYS
1	A	149	ASP
1	A	150	LEU
1	A	174	ASN
1	A	184	ASN
1	A	185	GLU
1	A	213	LEU
1	A	284	LYS
1	A	286	THR

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Mol	Chain	Res	Type
1	A	302	ASP
1	A	313	SER
1	A	359	ASN
1	A	361	SER
1	B	6	PRO
1	B	20	THR
1	B	41	LYS
1	B	61	ASP
1	B	69	LYS
1	B	90	THR
1	B	94	SER
1	B	149	ASP
1	B	184	ASN
1	B	185	GLU
1	B	235	LEU
1	B	273	LEU
1	B	286	THR
1	B	329	PRO
1	B	359	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	95	HIS
1	A	120	HIS
1	A	184	ASN
1	A	221	GLN
1	A	359	ASN
1	A	384	GLN
1	B	75	ASN
1	B	76	GLN
1	B	95	HIS
1	B	120	HIS
1	B	184	ASN
1	B	221	GLN
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	0.74	0	10,11,11	1.72	4 (40%)
2	XYL	B	400	3	9,9,9	1.05	1 (11%)	10,11,11	2.23	5 (50%)

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	C4-C3	-2.68	1.48	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	XYL	O5-C5-C4	-3.64	103.17	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	XYL	C1-C2-C3	-2.94	105.57	112.48
2	A	400	XYL	O2-C2-C1	-2.22	104.03	109.22
2	A	400	XYL	O4-C4-C5	-2.01	104.54	109.22
2	B	400	XYL	O3-C3-C4	2.03	113.87	108.75
2	A	400	XYL	C5-C4-C3	2.29	117.84	112.48
2	B	400	XYL	O2-C2-C3	2.34	114.89	109.02
2	A	400	XYL	O3-C3-C2	2.71	115.59	108.75
2	B	400	XYL	O1-C1-C2	2.98	117.58	111.10

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.