



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:55 pm BST

PDB ID : 1XLE  
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.

---

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

MolProbity	:	4.02b-467
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)	:	2.11

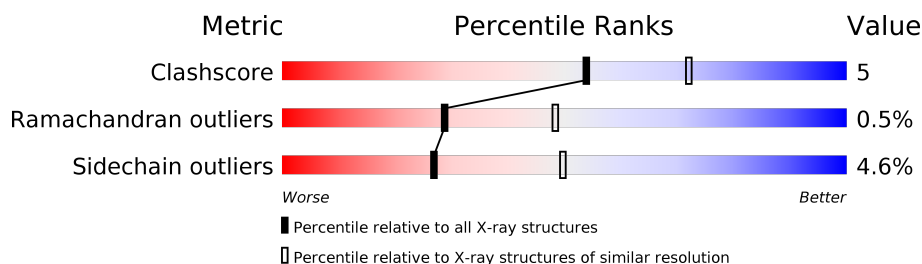
# 1 Overall quality at a glance

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

There are 3 unique types of molecules in this entry. The entry contains 6580 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 MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		

- Molecule 3 is water.

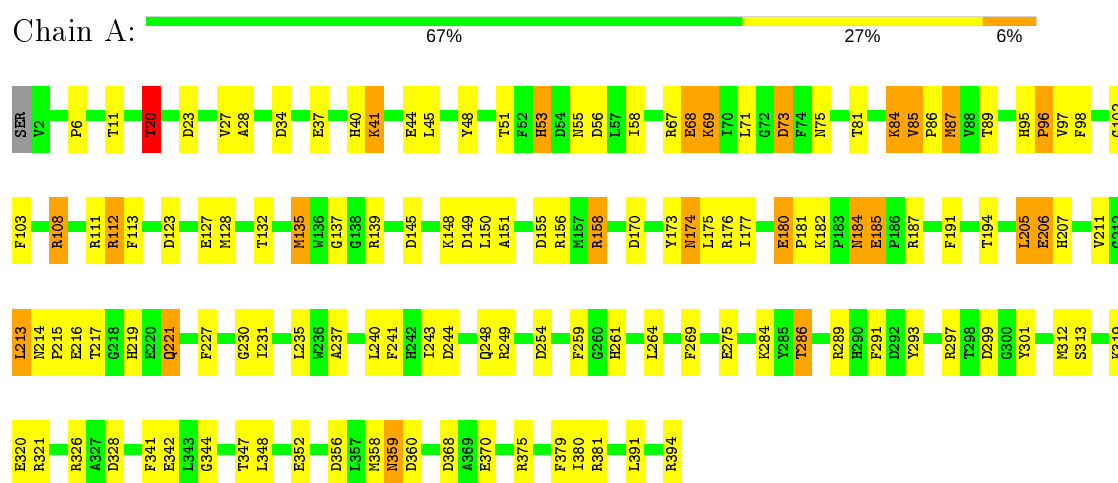
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	260	Total	O	0	0
			260	260		
3	B	262	Total	O	0	0
			262	262		

### 3 Residue-property plots

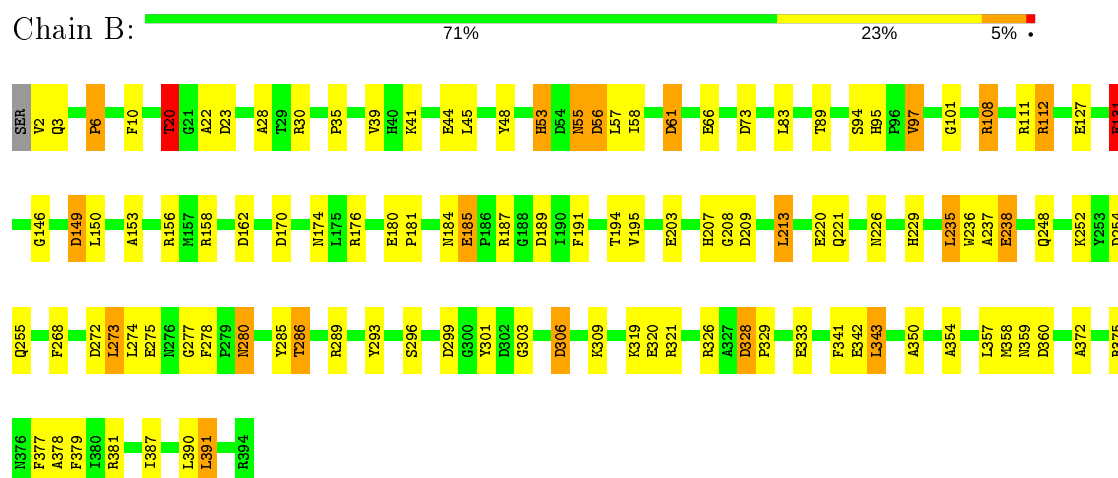
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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, $\alpha$ , $\beta$ , $\gamma$	105.40 Å   105.40 Å   154.00 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, $R_{free}$	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6580	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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

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	1.19	2/3101 (0.1%)	2.30	131/4204 (3.1%)
1	B	1.19	2/3101 (0.1%)	2.23	112/4204 (2.7%)
All	All	1.19	4/6202 (0.1%)	2.26	243/8408 (2.9%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	ARG	CD-NE	-9.06	1.31	1.46
1	A	158	ARG	CG-CD	-5.92	1.37	1.51
1	B	277	GLY	N-CA	5.36	1.54	1.46
1	B	112	ARG	CD-NE	-5.22	1.37	1.46

All (243) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ARG	CD-NE-CZ	36.39	174.55	123.60
1	A	158	ARG	CD-NE-CZ	26.02	160.03	123.60
1	A	112	ARG	CD-NE-CZ	25.59	159.42	123.60
1	A	289	ARG	CD-NE-CZ	20.48	152.28	123.60
1	A	394	ARG	NE-CZ-NH1	19.92	130.26	120.30
1	B	112	ARG	NE-CZ-NH2	19.10	129.85	120.30
1	B	293	TYR	CB-CG-CD2	-17.61	110.43	121.00
1	A	158	ARG	NE-CZ-NH2	-17.44	111.58	120.30
1	A	394	ARG	NE-CZ-NH2	-16.66	111.97	120.30
1	A	108	ARG	NE-CZ-NH1	16.30	128.45	120.30
1	B	187	ARG	NE-CZ-NH1	15.51	128.05	120.30
1	A	368	ASP	CB-CG-OD2	15.48	132.24	118.30
1	A	381	ARG	NE-CZ-NH1	14.80	127.70	120.30
1	A	394	ARG	CD-NE-CZ	14.41	143.77	123.60
1	B	108	ARG	NE-CZ-NH1	13.14	126.87	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ARG	CG-CD-NE	12.88	138.84	111.80
1	B	187	ARG	NE-CZ-NH2	-12.59	114.01	120.30
1	B	238	GLU	N-CA-CB	-12.52	88.06	110.60
1	B	299	ASP	CB-CG-OD1	12.24	129.32	118.30
1	A	187	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	A	127	GLU	N-CA-CB	11.99	132.18	110.60
1	B	108	ARG	NE-CZ-NH2	-11.95	114.32	120.30
1	B	293	TYR	CB-CG-CD1	11.87	128.12	121.00
1	A	176	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	187	ARG	NE-CZ-NH1	11.07	125.83	120.30
1	A	301	TYR	CB-CG-CD1	-10.87	114.48	121.00
1	B	23	ASP	CB-CG-OD2	10.58	127.82	118.30
1	B	20	THR	CA-CB-CG2	10.29	126.81	112.40
1	B	238	GLU	OE1-CD-OE2	-10.20	111.06	123.30
1	B	30	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	B	358	MET	C-N-CA	9.95	146.58	121.70
1	A	127	GLU	OE1-CD-OE2	-9.89	111.43	123.30
1	A	158	ARG	NE-CZ-NH1	9.89	125.24	120.30
1	A	241	PHE	CB-CG-CD1	9.80	127.66	120.80
1	B	149	ASP	CB-CG-OD1	9.78	127.10	118.30
1	B	379	PHE	CB-CG-CD1	9.77	127.64	120.80
1	B	238	GLU	CG-CD-OE2	9.75	137.81	118.30
1	B	278	PHE	CB-CG-CD1	9.72	127.61	120.80
1	B	213	LEU	CA-CB-CG	9.68	137.57	115.30
1	A	108	ARG	NE-CZ-NH2	-9.35	115.62	120.30
1	A	149	ASP	CB-CG-OD1	9.19	126.57	118.30
1	B	112	ARG	NE-CZ-NH1	-9.12	115.74	120.30
1	A	113	PHE	CB-CG-CD2	-9.12	114.42	120.80
1	A	127	GLU	CB-CA-C	-9.09	92.22	110.40
1	B	189	ASP	CB-CG-OD2	9.07	126.46	118.30
1	B	381	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	B	360	ASP	CB-CG-OD2	8.99	126.39	118.30
1	A	297	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	B	306	ASP	CB-CG-OD2	8.91	126.32	118.30
1	A	249	ARG	CD-NE-CZ	8.72	135.80	123.60
1	B	20	THR	N-CA-CB	-8.70	93.77	110.30
1	B	2	VAL	C-N-CA	8.67	143.37	121.70
1	B	278	PHE	CB-CG-CD2	-8.66	114.73	120.80
1	B	203	GLU	CG-CD-OE2	8.65	135.60	118.30
1	B	238	GLU	CB-CA-C	8.62	127.64	110.40
1	B	321	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	B	156	ARG	NE-CZ-NH1	8.58	124.59	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	ASP	CB-CG-OD1	8.52	125.97	118.30
1	A	359	ASN	CA-CB-CG	8.36	131.79	113.40
1	B	23	ASP	CB-CA-C	8.34	127.08	110.40
1	B	44	GLU	CG-CD-OE1	-8.29	101.72	118.30
1	B	189	ASP	CB-CG-OD1	-8.27	110.85	118.30
1	A	375	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	B	53	HIS	N-CA-CB	8.18	125.32	110.60
1	A	356	ASP	CB-CG-OD2	8.16	125.65	118.30
1	B	203	GLU	OE1-CD-OE2	-8.16	113.51	123.30
1	B	170	ASP	CB-CG-OD2	8.08	125.58	118.30
1	A	139	ARG	NE-CZ-NH2	8.07	124.34	120.30
1	A	23	ASP	CB-CG-OD1	8.04	125.53	118.30
1	A	123	ASP	CB-CG-OD1	7.96	125.46	118.30
1	A	51	THR	CA-CB-CG2	7.83	123.36	112.40
1	B	379	PHE	CB-CG-CD2	-7.70	115.41	120.80
1	A	87	MET	CA-CB-CG	7.62	126.26	113.30
1	A	67	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	B	56	ASP	CB-CG-OD2	7.56	125.11	118.30
1	A	360	ASP	CB-CG-OD2	7.54	125.09	118.30
1	A	73	ASP	CA-CB-CG	7.54	129.98	113.40
1	A	145	ASP	CB-CG-OD2	-7.54	111.52	118.30
1	A	249	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	B	273	LEU	CA-CB-CG	7.45	132.44	115.30
1	B	350	ALA	O-C-N	-7.39	110.63	123.20
1	B	176	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	180	GLU	CG-CD-OE1	7.31	132.92	118.30
1	A	342	GLU	CB-CA-C	-7.30	95.81	110.40
1	A	293	TYR	CB-CG-CD2	7.29	125.38	121.00
1	A	194	THR	CA-CB-CG2	7.26	122.56	112.40
1	A	123	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	B	391	LEU	C-N-CA	7.25	137.51	122.30
1	B	97	VAL	CA-CB-CG1	7.22	121.74	110.90
1	B	10	PHE	CB-CG-CD1	7.22	125.85	120.80
1	A	342	GLU	CA-CB-CG	7.18	129.20	113.40
1	A	368	ASP	OD1-CG-OD2	-7.16	109.70	123.30
1	A	127	GLU	CG-CD-OE1	7.16	132.61	118.30
1	A	23	ASP	CB-CA-C	7.14	124.69	110.40
1	A	326	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	A	342	GLU	N-CA-CB	7.11	123.40	110.60
1	A	170	ASP	CB-CG-OD2	-7.03	111.98	118.30
1	A	269	PHE	CB-CG-CD1	-7.01	115.89	120.80
1	A	145	ASP	CB-CG-OD1	6.96	124.56	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	GLU	CA-CB-CG	6.92	128.61	113.40
1	B	162	ASP	CB-CG-OD2	-6.91	112.09	118.30
1	B	111	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	170	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	113	PHE	CB-CG-CD1	6.87	125.61	120.80
1	A	299	ASP	CB-CG-OD1	6.83	124.44	118.30
1	B	326	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	B	372	ALA	O-C-N	-6.76	111.89	122.70
1	A	211	VAL	CA-CB-CG2	6.75	121.03	110.90
1	B	342	GLU	CG-CD-OE2	-6.67	104.95	118.30
1	B	372	ALA	CB-CA-C	6.65	120.07	110.10
1	A	53	HIS	CB-CA-C	-6.63	97.14	110.40
1	B	127	GLU	OE1-CD-OE2	-6.63	115.35	123.30
1	B	61	ASP	CB-CG-OD2	6.59	124.23	118.30
1	B	359	ASN	CA-CB-CG	6.58	127.88	113.40
1	A	173	TYR	CB-CG-CD1	6.57	124.94	121.00
1	B	22	ALA	CB-CA-C	6.53	119.90	110.10
1	B	286	THR	N-CA-CB	-6.52	97.91	110.30
1	B	23	ASP	OD1-CG-OD2	-6.49	110.97	123.30
1	A	139	ARG	NH1-CZ-NH2	-6.45	112.30	119.40
1	A	156	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	96	PRO	O-C-N	-6.43	112.41	122.70
1	A	261	HIS	C-N-CA	6.42	135.79	122.30
1	B	48	TYR	N-CA-CB	-6.41	99.06	110.60
1	A	135	MET	CG-SD-CE	6.40	110.44	100.20
1	B	289	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	176	ARG	NH1-CZ-NH2	-6.34	112.42	119.40
1	A	207	HIS	O-C-N	-6.34	112.43	123.20
1	A	352	GLU	CG-CD-OE2	6.32	130.94	118.30
1	B	194	THR	CA-CB-CG2	6.32	121.24	112.40
1	A	370	GLU	CG-CD-OE2	6.31	130.91	118.30
1	A	320	GLU	CG-CD-OE2	6.30	130.90	118.30
1	B	272	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	354	ALA	N-CA-CB	6.29	118.91	110.10
1	B	83	LEU	CA-CB-CG	6.28	129.75	115.30
1	A	98	PHE	CB-CG-CD2	-6.27	116.41	120.80
1	B	379	PHE	CA-CB-CG	6.25	128.90	113.90
1	B	209	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	321	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	127	GLU	CA-CB-CG	6.21	127.07	113.40
1	B	381	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	B	20	THR	CB-CA-C	6.21	128.35	111.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	THR	CA-CB-CG2	6.20	121.08	112.40
1	B	44	GLU	CG-CD-OE2	6.20	130.69	118.30
1	A	56	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	243	ILE	O-C-N	6.16	132.56	122.70
1	B	73	ASP	CA-CB-CG	6.15	126.93	113.40
1	B	343	LEU	CB-CG-CD2	-6.09	100.65	111.00
1	A	348	LEU	CA-CB-CG	6.08	129.29	115.30
1	B	301	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	A	156	ARG	CD-NE-CZ	6.03	132.05	123.60
1	B	236	TRP	CA-CB-CG	6.00	125.10	113.70
1	B	254	ASP	CB-CG-OD1	5.98	123.69	118.30
1	B	375	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	297	ARG	CG-CD-NE	5.93	124.24	111.80
1	A	139	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	6	PRO	C-N-CA	5.92	136.50	121.70
1	A	358	MET	C-N-CA	5.91	136.48	121.70
1	A	149	ASP	N-CA-C	-5.91	95.04	111.00
1	B	289	ARG	CD-NE-CZ	5.89	131.84	123.60
1	A	102	GLY	N-CA-C	-5.88	98.41	113.10
1	A	173	TYR	CB-CG-CD2	-5.85	117.49	121.00
1	B	101	GLY	O-C-N	5.84	133.13	123.20
1	A	155	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	73	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	274	LEU	CB-CG-CD1	-5.83	101.09	111.00
1	B	359	ASN	CB-CA-C	5.80	122.00	110.40
1	A	293	TYR	CB-CG-CD1	-5.79	117.53	121.00
1	A	128	MET	CA-C-N	5.78	127.75	116.20
1	B	255	GLN	CG-CD-OE1	-5.77	110.06	121.60
1	A	151	ALA	CB-CA-C	5.76	118.74	110.10
1	B	379	PHE	CB-CA-C	5.72	121.84	110.40
1	B	150	LEU	CB-CA-C	5.71	121.05	110.20
1	A	149	ASP	N-CA-CB	5.70	120.86	110.60
1	A	230	GLY	O-C-N	-5.66	113.64	122.70
1	B	187	ARG	CD-NE-CZ	5.66	131.52	123.60
1	A	205	LEU	CA-CB-CG	5.65	128.31	115.30
1	A	34	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	333	GLU	OE1-CD-OE2	5.64	130.07	123.30
1	A	216	GLU	OE1-CD-OE2	5.60	130.02	123.30
1	A	6	PRO	O-C-N	-5.59	113.75	122.70
1	A	286	THR	CA-C-N	5.59	127.38	116.20
1	A	291	PHE	CB-CG-CD1	5.56	124.69	120.80
1	A	244	ASP	CB-CG-OD2	-5.56	113.30	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	GLY	C-N-CA	5.54	135.55	121.70
1	A	137	GLY	C-N-CA	5.54	133.92	122.30
1	A	241	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	A	342	GLU	OE1-CD-OE2	5.51	129.91	123.30
1	B	254	ASP	CA-CB-CG	5.50	125.51	113.40
1	B	149	ASP	N-CA-C	-5.50	96.15	111.00
1	A	108	ARG	CD-NE-CZ	5.50	131.30	123.60
1	B	280	ASN	CA-C-N	5.50	127.20	116.20
1	A	237	ALA	C-N-CA	5.50	135.44	121.70
1	B	191	PHE	CB-CG-CD2	-5.49	116.96	120.80
1	B	236	TRP	N-CA-CB	5.48	120.46	110.60
1	A	297	ARG	CD-NE-CZ	5.46	131.25	123.60
1	B	350	ALA	CA-C-N	5.46	127.13	116.20
1	A	68	GLU	OE1-CD-OE2	5.44	129.83	123.30
1	B	235	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	A	264	LEU	CB-CA-C	5.43	120.52	110.20
1	B	320	GLU	OE1-CD-OE2	5.42	129.80	123.30
1	A	112	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	48	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	B	342	GLU	OE1-CD-OE2	5.40	129.78	123.30
1	A	379	PHE	CA-CB-CG	5.39	126.85	113.90
1	A	291	PHE	CB-CG-CD2	-5.39	117.03	120.80
1	A	243	ILE	CA-C-O	-5.36	108.86	120.10
1	A	381	ARG	NH1-CZ-NH2	-5.36	113.51	119.40
1	A	241	PHE	CG-CD1-CE1	5.35	126.69	120.80
1	B	185	GLU	CA-CB-CG	5.34	125.15	113.40
1	B	285	TYR	CD1-CE1-CZ	-5.32	115.01	119.80
1	A	67	ARG	CG-CD-NE	-5.31	100.64	111.80
1	A	175	LEU	CB-CA-C	-5.31	100.11	110.20
1	B	108	ARG	CD-NE-CZ	5.30	131.02	123.60
1	A	85	VAL	CG1-CB-CG2	-5.29	102.43	110.90
1	B	131	GLU	CG-CD-OE1	5.28	128.85	118.30
1	A	391	LEU	CA-CB-CG	5.25	127.39	115.30
1	A	27	VAL	CA-CB-CG2	5.25	118.77	110.90
1	B	328	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	259	PHE	C-N-CA	5.21	133.25	122.30
1	B	299	ASP	OD1-CG-OD2	-5.21	113.41	123.30
1	A	128	MET	O-C-N	-5.20	114.36	123.20
1	B	252	LYS	CA-CB-CG	5.19	124.81	113.40
1	B	97	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	B	207	HIS	CA-CB-CG	-5.18	104.79	113.60
1	B	358	MET	CG-SD-CE	5.18	108.49	100.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	GLY	C-N-CA	5.17	134.63	121.70
1	B	158	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	A	103	PHE	CB-CG-CD1	5.17	124.42	120.80
1	A	111	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	341	PHE	CB-CG-CD1	-5.12	117.22	120.80
1	B	174	ASN	C-N-CA	5.12	134.49	121.70
1	A	111	ARG	CA-CB-CG	5.09	124.61	113.40
1	B	55	ASN	CB-CA-C	5.09	120.59	110.40
1	A	254	ASP	CB-CA-C	5.09	120.57	110.40
1	A	213	LEU	CD1-CG-CD2	-5.06	95.33	110.50
1	B	153	ALA	CB-CA-C	5.04	117.66	110.10
1	A	301	TYR	CB-CG-CD2	5.03	124.02	121.00
1	A	347	THR	CA-CB-CG2	5.02	119.43	112.40
1	B	57	LEU	CB-CA-C	5.02	119.74	110.20
1	A	312	MET	CG-SD-CE	5.02	108.23	100.20
1	A	221	GLN	C-N-CA	5.01	134.23	121.70
1	B	55	ASN	C-N-CA	5.01	134.22	121.70
1	B	191	PHE	CB-CG-CD1	5.00	124.30	120.80

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	2882	35	0
1	B	3027	0	2880	29	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	260	0	0	5	1
3	B	262	0	0	4	1
All	All	6580	0	5762	62	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 5.

All (62) 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:61:ASP:OD1	3:B:427(B):HOH:O	1.71	1.05
1:A:75:ASN:ND2	3:A:599(A):HOH:O	2.12	0.83
1:B:238:GLU:OE1	3:B:710(B):HOH:O	2.03	0.76
1:A:206:GLU:HG2	3:A:803(A):HOH:O	1.86	0.76
1:A:95:HIS:HD2	1:A:97:VAL:H	1.40	0.70
1:A:174:ASN:HD22	1:A:174:ASN:N	1.92	0.67
1:A:206:GLU:CG	3:A:803(A):HOH:O	2.45	0.63
1:B:95:HIS:HD2	1:B:97:VAL:H	1.45	0.62
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.84	0.60
1:A:158:ARG:HG3	1:A:205:LEU:HD23	1.86	0.57
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.89	0.55
1:A:184:ASN:HD22	1:A:185:GLU:HB2	1.72	0.55
1:A:108:ARG:O	1:A:112:ARG:HG3	2.08	0.53
1:A:95:HIS:CD2	1:A:97:VAL:H	2.22	0.53
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.73	0.53
1:B:226:ASN:HB3	1:B:229:HIS:HB2	1.89	0.53
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.91	0.53
1:A:20:THR:HG23	1:A:28:ALA:CB	2.39	0.53
1:A:275:GLU:HG3	1:A:319:LYS:HG3	1.93	0.51
1:B:61:ASP:OD1	1:B:61:ASP:C	2.49	0.51
1:B:45:LEU:HD22	1:B:309:LYS:HG2	1.93	0.50
1:A:20:THR:HG23	1:A:28:ALA:HB1	1.93	0.50
1:B:55:ASN:HA	1:B:58:ILE:O	2.12	0.49
1:A:41:LYS:O	1:A:45:LEU:HG	2.13	0.49
1:A:174:ASN:N	1:A:174:ASN:ND2	2.61	0.48
1:B:61:ASP:OD1	1:B:61:ASP:O	2.30	0.48
1:A:58:ILE:HD11	1:A:71:LEU:HG	1.96	0.47
1:B:237:ALA:O	1:B:238:GLU:HB3	2.14	0.47
1:B:328:ASP:HA	1:B:329:PRO:HD2	1.75	0.47
1:A:135:MET:HE2	1:A:177:ILE:HD13	1.96	0.46
1:A:235:LEU:HG	1:A:240:LEU:HD23	1.97	0.46
1:A:84:LYS:HG3	1:A:85:VAL:N	2.31	0.46
1:B:280:ASN:OD1	1:B:341:PHE:HA	2.15	0.46
1:B:268:PHE:CD1	1:B:390:LEU:HD13	2.52	0.45
1:A:380:ILE:HD11	1:B:296:SER:H	1.81	0.45
1:A:69:LYS:HE2	1:A:73:ASP:OD2	2.16	0.45
1:B:53:HIS:O	1:B:56:ASP:HB2	2.16	0.45
1:B:180:GLU:HA	1:B:181:PRO:HD3	1.74	0.44
1:A:158:ARG:HB3	3:A:471(A):HOH:O	2.16	0.44
1:A:55:ASN:HA	1:A:58:ILE:O	2.18	0.44
1:A:217:THR:HA	1:A:227:PHE:CD1	2.53	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLY:HA2	1:B:306:ASP:HB2	1.99	0.44
1:B:387:ILE:O	1:B:391:LEU:HG	2.18	0.44
1:B:221:GLN:HE21	1:B:248:GLN:HB3	1.83	0.43
1:A:181:PRO:HA	3:A:484(A):HOH:O	2.18	0.43
1:B:35:PRO:O	1:B:39:VAL:HG23	2.19	0.43
1:B:208:GLY:HA3	3:B:602(B):HOH:O	2.19	0.43
1:B:195:VAL:HG13	1:B:213:LEU:HD11	2.01	0.43
1:B:195:VAL:HG23	1:B:220:GLU:CD	2.40	0.43
1:A:37:GLU:O	1:A:41:LYS:HB2	2.19	0.42
1:B:131:GLU:HG3	3:B:711(B):HOH:O	2.17	0.42
1:A:182:LYS:HD2	1:A:219:HIS:CE1	2.54	0.42
1:B:108:ARG:O	1:B:112:ARG:HG3	2.19	0.42
1:A:180:GLU:HG3	1:A:214:ASN:O	2.20	0.42
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.85	0.42
1:A:380:ILE:HD11	1:B:296:SER:N	2.34	0.42
1:B:53:HIS:HA	1:B:89:THR:O	2.20	0.42
1:B:377:PHE:O	1:B:378:ALA:HB3	2.21	0.41
1:A:87:MET:HA	1:A:132:THR:O	2.21	0.41
1:A:40:HIS:HA	1:A:81:THR:HG21	2.02	0.41
1:A:215:PRO:HG2	1:A:231:ILE:HG22	2.04	0.40
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.56	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:B:343:LEU:CD2	3:B:445(B):HOH:O[4_555]	1.93	0.27
3:A:472(A):HOH:O	3:A:722(A):HOH:O[4_555]	2.05	0.15

## 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%)	41	61
1	B	391/394 (99%)	372 (95%)	16 (4%)	3 (1%)	19	35
All	All	782/788 (99%)	746 (95%)	32 (4%)	4 (0%)	29	48

All (4) Ramachandran outliers are listed below:

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

### 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%)	23	44
1	B	305/310 (98%)	293 (96%)	12 (4%)	32	57
All	All	610/620 (98%)	582 (95%)	28 (5%)	27	50

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	41	LYS
1	A	44	GLU
1	A	68	GLU
1	A	69	LYS
1	A	84	LYS
1	A	96	PRO
1	A	150	LEU
1	A	174	ASN
1	A	184	ASN
1	A	206	GLU
1	A	213	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	284	LYS
1	A	286	THR
1	A	313	SER
1	A	359	ASN
1	B	6	PRO
1	B	20	THR
1	B	41	LYS
1	B	66	GLU
1	B	94	SER
1	B	131	GLU
1	B	149	ASP
1	B	184	ASN
1	B	235	LEU
1	B	273	LEU
1	B	286	THR
1	B	357	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	95	HIS
1	A	174	ASN
1	A	184	ASN
1	A	221	GLN
1	A	384	GLN
1	B	75	ASN
1	B	95	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 ⓘ

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, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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.