



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:55 pm BST

PDB ID : 1XLL  
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

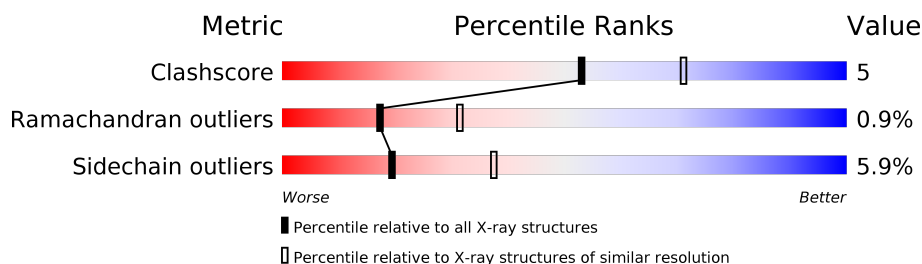
# 1 Overall quality at a glance

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 6583 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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	257	Total	O	0	0
			257	257		
3	B	268	Total	O	0	0
			268	268		

### 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



## 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   154.10 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, $R_{free}$	0.164 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6583	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	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: ZN

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	1.24	4/3101 (0.1%)	2.31	149/4204 (3.5%)
1	B	1.33	9/3101 (0.3%)	2.40	152/4204 (3.6%)
All	All	1.29	13/6202 (0.2%)	2.36	301/8408 (3.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	361	SER	CA-CB	-11.28	1.36	1.52
1	B	361	SER	CB-OG	8.31	1.53	1.42
1	B	216	GLU	CD-OE2	6.51	1.32	1.25
1	B	105	SER	CB-OG	6.04	1.50	1.42
1	A	282	GLY	N-CA	5.85	1.54	1.46
1	B	180	GLU	CD-OE1	-5.48	1.19	1.25
1	B	361	SER	C-N	-5.35	1.21	1.34
1	A	206	GLU	CD-OE2	5.31	1.31	1.25
1	B	220	GLU	CD-OE1	-5.25	1.19	1.25
1	A	105	SER	CB-OG	5.19	1.49	1.42
1	B	293	TYR	CG-CD1	5.17	1.45	1.39
1	B	374	GLU	CD-OE1	-5.17	1.20	1.25
1	A	313	SER	CB-OG	-5.13	1.35	1.42

All (301) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ARG	CD-NE-CZ	26.45	160.63	123.60
1	B	361	SER	C-N-CA	21.76	176.11	121.70
1	B	358	MET	C-N-CA	20.94	174.06	121.70
1	B	361	SER	N-CA-CB	20.25	140.87	110.50
1	B	108	ARG	NE-CZ-NH1	19.45	130.02	120.30
1	A	112	ARG	NE-CZ-NH1	18.87	129.74	120.30
1	A	249	ARG	NE-CZ-NH1	17.54	129.07	120.30
1	B	381	ARG	NE-CZ-NH2	-17.49	111.55	120.30
1	A	394	ARG	CD-NE-CZ	16.40	146.56	123.60
1	B	360	ASP	CA-C-N	16.21	152.86	117.20
1	A	289	ARG	CD-NE-CZ	14.72	144.21	123.60
1	A	108	ARG	NE-CZ-NH1	14.43	127.52	120.30
1	B	381	ARG	NE-CZ-NH1	13.93	127.26	120.30
1	B	108	ARG	NE-CZ-NH2	-13.80	113.40	120.30
1	A	23	ASP	CB-CG-OD1	13.62	130.56	118.30
1	B	256	ASP	CB-CG-OD1	13.56	130.50	118.30
1	B	359	ASN	C-N-CA	13.37	155.13	121.70
1	B	333	GLU	OE1-CD-OE2	13.21	139.16	123.30
1	B	249	ARG	NE-CZ-NH1	12.86	126.73	120.30
1	A	113	PHE	CB-CG-CD2	-12.40	112.12	120.80
1	A	241	PHE	CB-CG-CD1	12.20	129.34	120.80
1	A	249	ARG	NE-CZ-NH2	-12.14	114.23	120.30
1	B	357	LEU	O-C-N	-11.88	103.70	122.70
1	B	360	ASP	CB-CG-OD2	11.72	128.85	118.30
1	B	342	GLU	OE1-CD-OE2	11.71	137.36	123.30
1	B	297	ARG	NE-CZ-NH2	11.70	126.15	120.30
1	B	112	ARG	CD-NE-CZ	11.59	139.82	123.60
1	A	158	ARG	CD-NE-CZ	11.31	139.43	123.60
1	B	299	ASP	CB-CG-OD1	11.11	128.30	118.30
1	B	358	MET	CA-C-O	11.05	143.31	120.10
1	B	249	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	B	361	SER	CB-CA-C	-10.80	89.57	110.10
1	A	111	ARG	NE-CZ-NH2	-10.69	114.95	120.30
1	B	30	ARG	NE-CZ-NH1	10.63	125.61	120.30
1	B	328	ASP	CB-CG-OD1	10.48	127.73	118.30
1	A	80	ASP	CB-CG-OD1	10.42	127.68	118.30
1	B	213	LEU	CA-CB-CG	10.34	139.09	115.30
1	B	358	MET	N-CA-CB	10.22	128.99	110.60
1	A	149	ASP	CB-CG-OD1	10.12	127.41	118.30
1	B	360	ASP	O-C-N	-10.07	106.59	122.70
1	B	44	GLU	CA-CB-CG	10.05	135.51	113.40
1	B	394	ARG	NE-CZ-NH2	-10.03	115.29	120.30
1	A	156	ARG	NE-CZ-NH1	10.00	125.30	120.30

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	LEU	CA-C-N	9.97	139.12	117.20
1	B	209	ASP	CB-CG-OD2	9.94	127.25	118.30
1	B	342	GLU	CG-CD-OE2	-9.89	98.52	118.30
1	A	381	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	B	23	ASP	CB-CG-OD2	9.77	127.10	118.30
1	A	108	ARG	NE-CZ-NH2	-9.75	115.42	120.30
1	B	379	PHE	CB-CG-CD1	9.47	127.43	120.80
1	A	328	ASP	CB-CG-OD1	9.42	126.78	118.30
1	A	34	ASP	CB-CG-OD2	9.36	126.72	118.30
1	B	360	ASP	CA-C-O	-9.35	100.47	120.10
1	B	357	LEU	C-N-CA	9.30	144.95	121.70
1	B	364	PHE	O-C-N	-9.00	108.30	122.70
1	B	67	ARG	CG-CD-NE	8.90	130.49	111.80
1	B	379	PHE	CB-CG-CD2	-8.86	114.60	120.80
1	B	293	TYR	CB-CG-CD2	-8.77	115.74	121.00
1	B	20	THR	CA-CB-CG2	8.67	124.54	112.40
1	B	108	ARG	CD-NE-CZ	8.66	135.72	123.60
1	B	358	MET	O-C-N	-8.59	108.95	122.70
1	B	359	ASN	CB-CA-C	8.55	127.50	110.40
1	A	333	GLU	CA-CB-CG	8.51	132.12	113.40
1	A	342	GLU	CA-CB-CG	8.42	131.92	113.40
1	A	6	PRO	C-N-CA	8.40	142.70	121.70
1	B	306	ASP	CB-CG-OD2	8.28	125.75	118.30
1	A	272	ASP	CB-CG-OD1	-8.20	110.92	118.30
1	B	254	ASP	CB-CG-OD2	8.18	125.67	118.30
1	B	273	LEU	CA-CB-CG	8.15	134.06	115.30
1	A	375	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	B	358	MET	CA-CB-CG	-8.12	99.50	113.30
1	A	113	PHE	CB-CG-CD1	8.10	126.47	120.80
1	A	394	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	B	350	ALA	N-CA-CB	8.06	121.38	110.10
1	B	2	VAL	CA-CB-CG2	8.02	122.92	110.90
1	A	149	ASP	N-CA-CB	8.01	125.01	110.60
1	A	394	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	B	297	ARG	NE-CZ-NH1	-7.98	116.31	120.30
1	A	80	ASP	CB-CG-OD2	-7.95	111.15	118.30
1	A	241	PHE	CB-CG-CD2	-7.91	115.26	120.80
1	A	170	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	A	68	GLU	OE1-CD-OE2	7.83	132.70	123.30
1	B	187	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	A	360	ASP	CB-CG-OD2	7.73	125.25	118.30
1	A	84	LYS	CA-CB-CG	7.70	130.34	113.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ARG	NE-CZ-NH2	7.69	124.15	120.30
1	B	20	THR	N-CA-CB	-7.61	95.85	110.30
1	A	306	ASP	CB-CG-OD2	7.60	125.14	118.30
1	B	278	PHE	CB-CG-CD2	-7.58	115.49	120.80
1	A	320	GLU	CA-CB-CG	7.51	129.93	113.40
1	B	362	ALA	CB-CA-C	7.50	121.35	110.10
1	A	123	ASP	CB-CG-OD1	7.39	124.96	118.30
1	A	194	THR	CA-CB-CG2	7.37	122.72	112.40
1	A	127	GLU	CA-CB-CG	7.36	129.59	113.40
1	A	144	TYR	CB-CG-CD2	-7.36	116.59	121.00
1	A	8	ASP	CB-CG-OD2	7.35	124.92	118.30
1	A	342	GLU	CB-CA-C	-7.35	95.69	110.40
1	A	293	TYR	CB-CG-CD1	-7.32	116.61	121.00
1	A	68	GLU	CA-CB-CG	-7.32	97.30	113.40
1	B	30	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	34	ASP	OD1-CG-OD2	-7.31	109.41	123.30
1	A	127	GLU	N-CA-CB	7.30	123.74	110.60
1	B	23	ASP	OD1-CG-OD2	-7.29	109.45	123.30
1	A	315	TYR	CB-CG-CD2	-7.25	116.65	121.00
1	A	176	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	289	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	B	362	ALA	CA-C-O	-7.23	104.91	120.10
1	A	27	VAL	CA-CB-CG2	7.18	121.67	110.90
1	B	127	GLU	OE1-CD-OE2	-7.17	114.69	123.30
1	A	269	PHE	CB-CG-CD1	-7.15	115.80	120.80
1	A	315	TYR	CB-CG-CD1	7.11	125.27	121.00
1	A	84	LYS	N-CA-CB	-7.10	97.81	110.60
1	A	6	PRO	O-C-N	-7.08	111.37	122.70
1	A	320	GLU	CG-CD-OE2	7.06	132.43	118.30
1	A	368	ASP	CB-CG-OD1	7.05	124.64	118.30
1	A	23	ASP	CB-CA-C	6.99	124.38	110.40
1	A	342	GLU	N-CA-CB	6.93	123.07	110.60
1	A	297	ARG	CG-CD-NE	6.92	126.33	111.80
1	A	249	ARG	CD-NE-CZ	6.90	133.26	123.60
1	B	279	PRO	O-C-N	-6.90	111.66	122.70
1	A	393	SER	C-N-CA	6.86	138.86	121.70
1	A	53	HIS	N-CA-CB	6.85	122.92	110.60
1	A	176	ARG	NH1-CZ-NH2	-6.83	111.88	119.40
1	A	256	ASP	CB-CG-OD2	6.83	124.45	118.30
1	A	301	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	B	363	SER	CB-CA-C	6.82	123.05	110.10
1	A	112	ARG	NH1-CZ-NH2	-6.82	111.90	119.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ASP	CB-CG-OD1	6.75	124.38	118.30
1	B	187	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	362	ALA	N-CA-C	-6.74	92.81	111.00
1	B	127	GLU	CG-CD-OE2	6.73	131.76	118.30
1	B	154	LEU	CB-CA-C	6.72	122.97	110.20
1	B	23	ASP	CB-CA-C	6.71	123.83	110.40
1	B	170	ASP	CB-CG-OD2	6.71	124.34	118.30
1	A	143	GLU	OE1-CD-OE2	-6.71	115.25	123.30
1	A	352	GLU	OE1-CD-OE2	-6.70	115.26	123.30
1	B	362	ALA	CA-C-N	6.69	131.93	117.20
1	B	206	GLU	CA-CB-CG	6.68	128.09	113.40
1	B	361	SER	CA-C-O	6.65	134.07	120.10
1	B	301	TYR	CB-CG-CD1	-6.64	117.01	121.00
1	B	256	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	A	181	PRO	O-C-N	6.60	133.25	122.70
1	B	370	GLU	OE1-CD-OE2	6.58	131.20	123.30
1	B	292	ASP	CB-CG-OD2	6.57	124.22	118.30
1	A	374	GLU	OE1-CD-OE2	6.57	131.18	123.30
1	B	189	ASP	CB-CG-OD2	6.57	124.21	118.30
1	A	359	ASN	CA-CB-CG	6.56	127.84	113.40
1	B	392	GLY	C-N-CA	6.55	138.09	121.70
1	B	74	PHE	CB-CG-CD2	-6.52	116.24	120.80
1	A	239	LYS	CA-CB-CG	6.45	127.58	113.40
1	B	82	GLY	CA-C-O	-6.43	109.03	120.60
1	A	391	LEU	C-N-CA	6.41	135.77	122.30
1	A	238	GLU	OE1-CD-OE2	6.41	130.99	123.30
1	B	343	LEU	C-N-CA	6.37	135.68	122.30
1	A	51	THR	CA-CB-CG2	6.36	121.30	112.40
1	B	273	LEU	CB-CG-CD1	6.34	121.79	111.00
1	A	145	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	A	135	MET	CG-SD-CE	6.26	110.22	100.20
1	A	118	VAL	CA-CB-CG1	6.26	120.29	110.90
1	B	244	ASP	N-CA-CB	6.26	121.86	110.60
1	B	249	ARG	CA-C-N	6.25	128.70	116.20
1	A	53	HIS	CB-CA-C	-6.23	97.93	110.40
1	A	123	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	B	143	GLU	OE1-CD-OE2	-6.20	115.86	123.30
1	A	293	TYR	CB-CG-CD2	6.20	124.72	121.00
1	A	34	ASP	CB-CG-OD1	6.18	123.87	118.30
1	A	156	ARG	CD-NE-CZ	6.15	132.21	123.60
1	B	249	ARG	O-C-N	-6.13	112.78	123.20
1	B	97	VAL	CA-CB-CG1	6.10	120.05	110.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	PHE	CB-CG-CD1	-6.10	116.53	120.80
1	A	167	TYR	CA-C-N	6.09	130.60	117.20
1	B	127	GLU	CA-CB-CG	6.06	126.74	113.40
1	B	357	LEU	N-CA-C	-6.06	94.64	111.00
1	A	189	ASP	CB-CG-OD2	6.04	123.73	118.30
1	B	79	LYS	O-C-N	-6.02	113.07	122.70
1	A	149	ASP	N-CA-C	-6.01	94.76	111.00
1	A	167	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	A	145	ASP	CB-CG-OD1	6.01	123.71	118.30
1	B	278	PHE	CB-CG-CD1	6.00	125.00	120.80
1	B	388	GLU	O-C-N	-5.99	113.11	122.70
1	B	54	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	B	286	THR	N-CA-CB	-5.98	98.94	110.30
1	B	53	HIS	N-CA-CB	5.97	121.35	110.60
1	A	348	LEU	CA-CB-CG	5.97	129.04	115.30
1	A	73	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	A	299	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	211	VAL	CA-CB-CG2	5.94	119.81	110.90
1	A	84	LYS	CG-CD-CE	5.92	129.65	111.90
1	A	137	GLY	C-N-CA	5.92	134.72	122.30
1	A	222	MET	C-N-CA	5.91	136.48	121.70
1	A	30	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	B	333	GLU	CG-CD-OE2	-5.89	106.52	118.30
1	A	341	PHE	CB-CG-CD1	-5.89	116.68	120.80
1	B	301	TYR	CB-CG-CD2	5.88	124.53	121.00
1	B	60	PHE	C-N-CA	5.86	136.36	121.70
1	B	149	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	85	VAL	CG1-CB-CG2	-5.85	101.55	110.90
1	A	368	ASP	OD1-CG-OD2	-5.83	112.22	123.30
1	A	20	THR	N-CA-CB	-5.82	99.25	110.30
1	A	56	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	363	SER	O-C-N	-5.80	113.42	122.70
1	B	206	GLU	OE1-CD-OE2	-5.80	116.34	123.30
1	B	151	ALA	O-C-N	-5.79	113.43	122.70
1	B	154	LEU	CA-CB-CG	5.78	128.60	115.30
1	A	255	GLN	CA-C-O	5.75	132.17	120.10
1	B	88	VAL	CG1-CB-CG2	-5.74	101.72	110.90
1	A	205	LEU	CA-CB-CG	5.74	128.50	115.30
1	B	328	ASP	OD1-CG-OD2	-5.73	112.41	123.30
1	A	286	THR	CA-C-N	5.73	127.65	116.20
1	B	23	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	375	ARG	NE-CZ-NH2	-5.72	117.44	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	137	GLY	C-N-CA	5.68	134.23	122.30
1	B	19	TRP	N-CA-CB	5.68	120.82	110.60
1	B	98	PHE	CB-CG-CD2	-5.68	116.82	120.80
1	B	28	ALA	CB-CA-C	-5.67	101.60	110.10
1	B	110	ILE	CB-CG1-CD1	5.66	129.75	113.90
1	A	56	ASP	CB-CG-OD1	-5.66	113.21	118.30
1	A	297	ARG	CA-CB-CG	5.66	125.84	113.40
1	B	37	GLU	CB-CG-CD	5.65	129.45	114.20
1	A	309	LYS	CA-CB-CG	5.64	125.80	113.40
1	B	361	SER	O-C-N	-5.63	113.69	122.70
1	B	30	ARG	CG-CD-NE	5.63	123.63	111.80
1	A	341	PHE	CB-CG-CD2	5.62	124.73	120.80
1	A	292	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	3	GLN	CB-CA-C	5.61	121.62	110.40
1	A	235	LEU	O-C-N	-5.61	113.73	122.70
1	B	293	TYR	CG-CD2-CE2	-5.60	116.82	121.30
1	B	134	VAL	CA-CB-CG1	5.58	119.27	110.90
1	A	48	TYR	CB-CG-CD2	5.58	124.35	121.00
1	B	354	ALA	N-CA-CB	5.58	117.91	110.10
1	B	372	ALA	O-C-N	-5.57	113.79	122.70
1	B	48	TYR	CB-CG-CD1	-5.56	117.66	121.00
1	B	347	THR	CA-CB-CG2	5.55	120.17	112.40
1	A	370	GLU	CG-CD-OE1	-5.55	107.20	118.30
1	B	149	ASP	N-CA-C	-5.52	96.09	111.00
1	B	279	PRO	C-N-CA	5.51	135.47	121.70
1	B	20	THR	CB-CA-C	5.48	126.41	111.60
1	A	167	TYR	O-C-N	-5.48	113.94	122.70
1	A	244	ASP	CA-CB-CG	5.48	125.45	113.40
1	B	56	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	242	HIS	CA-CB-CG	5.46	122.88	113.60
1	B	189	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	B	32	ASN	CA-CB-CG	-5.42	101.48	113.40
1	A	223	ALA	CB-CA-C	-5.42	101.97	110.10
1	A	96	PRO	O-C-N	-5.41	114.04	122.70
1	A	176	ARG	CD-NE-CZ	5.41	131.18	123.60
1	A	301	TYR	CB-CG-CD1	5.41	124.24	121.00
1	A	192	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	167	TYR	CB-CG-CD1	5.39	124.23	121.00
1	B	73	ASP	CA-CB-CG	5.39	125.25	113.40
1	A	7	ALA	C-N-CA	5.38	135.16	121.70
1	B	263	ASP	CB-CG-OD2	5.38	123.14	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	PRO	C-N-CA	5.38	135.14	121.70
1	B	236	TRP	CA-CB-CG	5.36	123.89	113.70
1	A	386	ALA	CB-CA-C	5.36	118.14	110.10
1	B	238	GLU	CB-CG-CD	5.36	128.66	114.20
1	A	215	PRO	O-C-N	5.35	131.27	122.70
1	B	254	ASP	CB-CA-C	5.33	121.06	110.40
1	A	368	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	379	PHE	CB-CA-C	5.33	121.06	110.40
1	A	14	LEU	CA-C-O	5.31	131.24	120.10
1	B	216	GLU	CG-CD-OE1	5.27	128.84	118.30
1	B	48	TYR	N-CA-CB	-5.24	101.16	110.60
1	A	291	PHE	CB-CG-CD1	5.23	124.46	120.80
1	A	372	ALA	O-C-N	-5.20	114.38	122.70
1	B	191	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	B	174	ASN	C-N-CA	5.19	134.67	121.70
1	A	391	LEU	CA-CB-CG	5.19	127.23	115.30
1	B	360	ASP	N-CA-CB	5.18	119.92	110.60
1	B	299	ASP	OD1-CG-OD2	-5.18	113.46	123.30
1	B	7	ALA	CA-C-O	-5.16	109.25	120.10
1	A	207	HIS	O-C-N	-5.15	114.44	123.20
1	B	348	LEU	CA-CB-CG	5.15	127.16	115.30
1	A	107	ASP	CA-CB-CG	5.15	124.72	113.40
1	A	158	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	110	ILE	O-C-N	-5.14	114.47	122.70
1	B	162	ASP	CB-CG-OD1	5.14	122.93	118.30
1	B	363	SER	N-CA-CB	-5.13	102.80	110.50
1	A	48	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	B	192	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	109	SER	CB-CA-C	5.11	119.80	110.10
1	B	225	LEU	CA-CB-CG	5.10	127.04	115.30
1	A	187	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	357	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	A	8	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	B	254	ASP	CA-CB-CG	5.09	124.59	113.40
1	B	220	GLU	OE1-CD-OE2	5.09	129.40	123.30
1	A	103	PHE	CB-CG-CD1	5.08	124.35	120.80
1	B	391	LEU	C-N-CA	5.08	132.96	122.30
1	A	102	GLY	N-CA-C	-5.07	100.43	113.10
1	A	173	TYR	CB-CG-CD1	5.05	124.03	121.00
1	A	297	ARG	O-C-N	-5.05	114.63	122.70
1	B	219	HIS	CA-C-N	5.04	128.29	117.20
1	A	353	SER	O-C-N	5.03	130.75	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	THR	C-N-CA	5.03	134.27	121.70
1	A	289	ARG	N-CA-CB	5.02	119.64	110.60
1	A	390	LEU	C-N-CA	5.02	134.25	121.70
1	A	44	GLU	CG-CD-OE2	5.01	128.31	118.30
1	B	294	LYS	CB-CA-C	-5.01	100.39	110.40
1	B	372	ALA	CB-CA-C	5.00	117.60	110.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	359	ASN	Mainchain
1	B	362	ALA	Mainchain
1	B	364	PHE	Mainchain

## 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	31	1
1	B	3027	0	2876	33	12
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	257	0	0	4	0
3	B	268	0	0	3	5
All	All	6583	0	5756	64	12

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 (64) 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:357:LEU:HG	1:B:359:ASN:HA	1.66	0.75
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.67	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLU:HG3	1:A:319:LYS:HG3	1.76	0.68
1:B:95:HIS:HD2	1:B:97:VAL:H	1.41	0.66
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.81	0.63
1:B:361:SER:HB3	1:B:366:GLY:H	1.62	0.63
1:A:158:ARG:HG3	1:A:205:LEU:HD23	1.79	0.63
1:A:95:HIS:HD2	1:A:97:VAL:H	1.48	0.61
1:A:215:PRO:HG2	1:A:231:ILE:HG22	1.85	0.58
1:B:361:SER:CB	1:B:366:GLY:H	2.17	0.58
1:B:131:GLU:HG3	3:B:649(B):HOH:O	2.04	0.58
1:A:84:LYS:HB2	3:A:660(A):HOH:O	2.03	0.57
1:A:43:ALA:HB2	1:A:83:LEU:HD13	1.90	0.54
1:A:20:THR:HG23	1:A:28:ALA:CB	2.38	0.54
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.91	0.53
1:A:277:GLY:HA3	1:A:284:LYS:HD3	1.91	0.52
1:B:45:LEU:HB3	1:B:309:LYS:HE3	1.90	0.52
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.76	0.51
1:A:69:LYS:HE2	1:A:73:ASP:OD2	2.11	0.50
1:B:361:SER:HB2	1:B:365:ALA:N	2.27	0.50
1:B:361:SER:CB	1:B:364:PHE:H	2.25	0.50
1:B:364:PHE:HB3	3:B:539(B):HOH:O	2.11	0.49
1:A:242:HIS:CD2	1:A:288:PRO:HG2	2.48	0.48
1:B:45:LEU:HD22	1:B:309:LYS:CD	2.43	0.48
1:B:357:LEU:O	1:B:360:ASP:N	2.45	0.48
1:B:53:HIS:HA	1:B:89:THR:O	2.12	0.48
1:A:235:LEU:HG	1:A:240:LEU:HD23	1.96	0.47
1:A:328:ASP:HA	1:A:329:PRO:HD3	1.75	0.46
1:B:63:THR:HG23	1:B:66:GLU:OE2	2.15	0.46
1:A:246:ASN:HB2	1:A:257:LEU:O	2.16	0.46
1:A:55:ASN:HA	1:A:58:ILE:O	2.16	0.46
1:A:87:MET:HA	1:A:132:THR:O	2.16	0.45
1:A:20:THR:HG23	1:A:28:ALA:HB1	1.98	0.45
1:B:226:ASN:HB3	1:B:229:HIS:HB2	1.98	0.45
1:A:158:ARG:HB3	3:A:459(A):HOH:O	2.17	0.45
1:B:23:ASP:HB2	1:B:24:PRO:HD2	1.99	0.45
1:B:67:ARG:HG3	1:B:71:LEU:HD12	1.99	0.45
1:B:10:PHE:CD2	1:B:312:MET:HG2	2.51	0.45
1:B:62:ALA:HA	1:B:66:GLU:OE1	2.18	0.44
1:A:35:PRO:O	1:A:39:VAL:HG23	2.17	0.44
1:A:120:HIS:O	1:A:123:ASP:HB2	2.17	0.44
1:A:75:ASN:ND2	3:A:561(A):HOH:O	2.50	0.44
1:B:278:PHE:HA	1:B:279:PRO:HD3	1.88	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ARG:O	1:B:252:LYS:HE3	2.18	0.43
1:B:357:LEU:HD23	1:B:359:ASN:ND2	2.32	0.43
1:A:95:HIS:CD2	1:A:97:VAL:H	2.33	0.43
1:A:19:TRP:CE3	1:A:294:LYS:HB3	2.53	0.43
1:A:20:THR:HG23	1:A:28:ALA:HB2	2.00	0.43
1:A:20:THR:HB	3:A:546(A):HOH:O	2.17	0.43
1:A:331:VAL:O	1:A:335:MET:HG3	2.19	0.43
1:A:133:PHE:O	1:A:177:ILE:HA	2.19	0.43
1:B:238:GLU:HG3	3:B:647(B):HOH:O	2.19	0.42
1:B:360:ASP:O	1:B:363:SER:N	2.52	0.42
1:B:354:ALA:O	1:B:358:MET:N	2.52	0.42
1:B:256:ASP:HB3	1:B:293:TYR:HA	2.02	0.42
1:A:58:ILE:HA	1:A:59:PRO:HD3	1.81	0.42
1:B:79:LYS:O	1:B:80:ASP:C	2.59	0.42
1:A:231:ILE:O	1:A:235:LEU:HB2	2.21	0.41
1:B:3:GLN:HA	1:B:4:PRO:HD2	1.95	0.41
1:B:42:LEU:HD23	1:B:42:LEU:HA	1.96	0.41
1:A:174:ASN:HD22	1:A:174:ASN:N	2.19	0.41
1:A:180:GLU:HA	1:A:181:PRO:HD3	1.78	0.40
1:B:11:THR:HG21	1:B:86:PRO:HG2	2.02	0.40
1:B:55:ASN:HA	1:B:58:ILE:O	2.22	0.40

All (12) 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:105:SER:N	3:B:592(B):HOH:O[4_555]	1.17	1.03
1:B:116:ALA:N	1:B:359:ASN:OD1[4_555]	1.20	1.00
1:B:116:ALA:CB	1:B:359:ASN:CB[4_555]	1.30	0.90
1:B:116:ALA:CA	1:B:359:ASN:OD1[4_555]	1.35	0.85
1:B:104:THR:C	3:B:592(B):HOH:O[4_555]	1.38	0.82
1:B:105:SER:CA	3:B:592(B):HOH:O[4_555]	1.70	0.50
1:B:116:ALA:CA	1:B:359:ASN:CG[4_555]	1.76	0.44
1:B:115:LEU:C	1:B:359:ASN:OD1[4_555]	1.86	0.34
1:B:104:THR:O	3:B:592(B):HOH:O[4_555]	1.92	0.28
1:B:116:ALA:CA	1:B:359:ASN:CB[4_555]	2.01	0.19
1:B:343:LEU:CD2	3:B:438(B):HOH:O[4_555]	2.11	0.09
1:A:69:LYS:NZ	1:B:276:ASN:O[6_665]	2.14	0.06



## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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%)	366 (94%)	19 (5%)	6 (2%)	10	18
All	All	782/788 (99%)	740 (95%)	35 (4%)	7 (1%)	17	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	358	MET
1	B	359	ASN
1	B	360	ASP
1	A	185	GLU
1	B	185	GLU
1	B	3	GLN
1	B	23	ASP

### 5.3.2 Protein sidechains [i](#)

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%)	287 (94%)	18 (6%)	19	37
1	B	305/310 (98%)	287 (94%)	18 (6%)	19	37
All	All	610/620 (98%)	574 (94%)	36 (6%)	19	37

All (36) 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	90	THR
1	A	94	SER
1	A	96	PRO
1	A	150	LEU
1	A	158	ARG
1	A	174	ASN
1	A	184	ASN
1	A	213	LEU
1	A	235	LEU
1	A	284	LYS
1	A	286	THR
1	A	359	ASN
1	B	6	PRO
1	B	20	THR
1	B	41	LYS
1	B	44	GLU
1	B	59	PRO
1	B	66	GLU
1	B	94	SER
1	B	131	GLU
1	B	184	ASN
1	B	213	LEU
1	B	235	LEU
1	B	273	LEU
1	B	286	THR
1	B	293	TYR
1	B	333	GLU
1	B	358	MET
1	B	359	ASN
1	B	360	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	95	HIS
1	A	120	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	174	ASN
1	A	184	ASN
1	A	221	GLN
1	A	384	GLN
1	B	75	ASN
1	B	76	GLN
1	B	95	HIS
1	B	221	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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 ⓘ

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.