



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:56 pm BST

PDB ID : 1XLB
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

<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

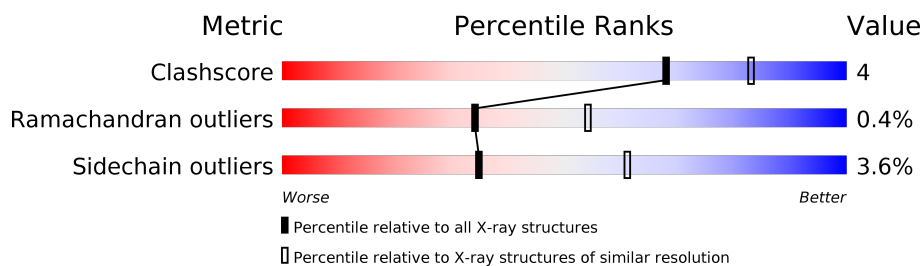
1 Overall quality at a glance

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 ≥ 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 6640 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
			3026	1919	521	577	9			
1	B	393	Total	C	N	O	S	0	0	0
			3026	1919	521	577	9			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

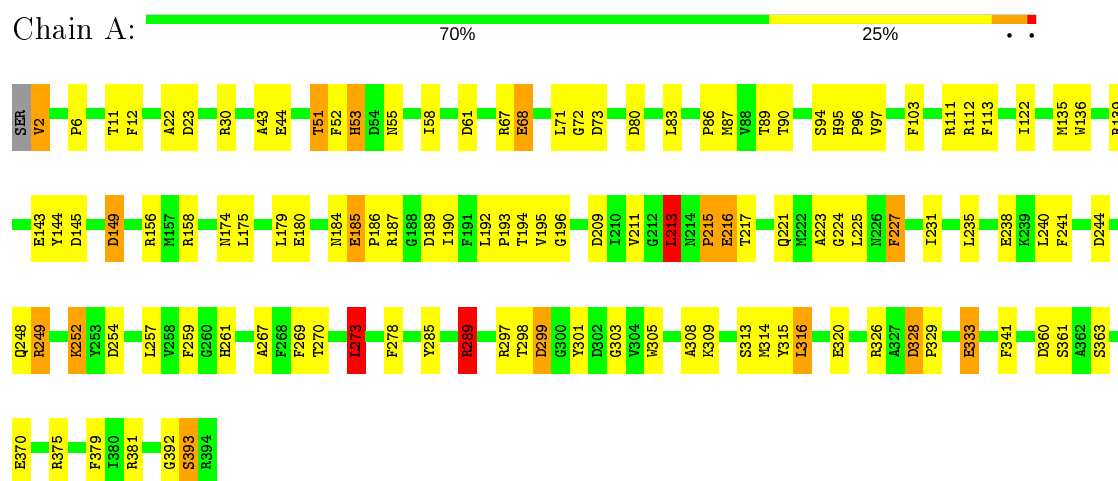
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	298	Total	O	0	0
			298	298		
3	B	288	Total	O	0	0
			288	288		

3 Residue-property plots

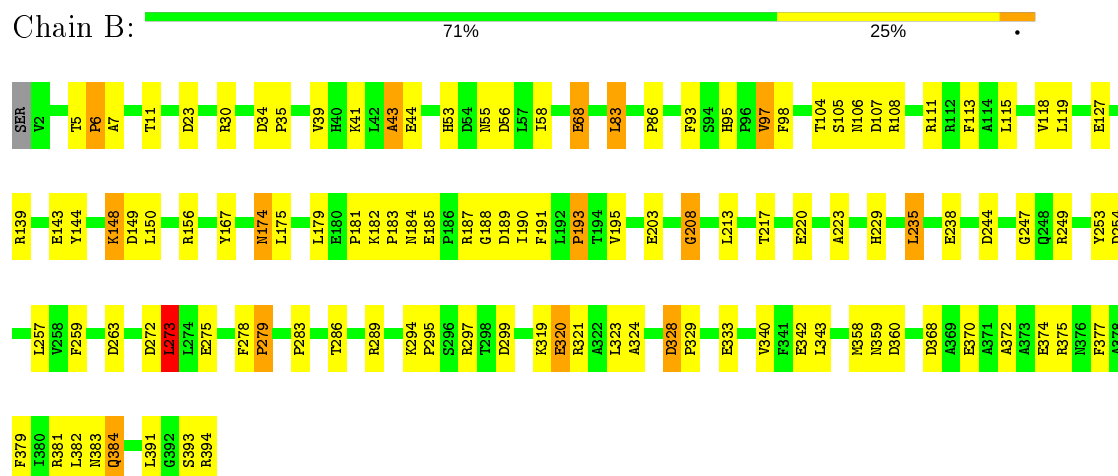
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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, α , β , γ	105.30 Å 105.30 Å 153.50 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}	0.157 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6640	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.05	0/3100	2.10	125/4201 (3.0%)
1	B	1.04	1/3100 (0.0%)	2.18	132/4201 (3.1%)
All	All	1.04	1/6200 (0.0%)	2.15	257/8402 (3.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	220	GLU	CD-OE1	-5.20	1.20	1.25

All (257) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	ARG	CD-NE-CZ	18.44	149.41	123.60
1	B	379	PHE	CB-CG-CD2	17.92	133.34	120.80
1	A	381	ARG	NE-CZ-NH1	17.21	128.91	120.30
1	B	375	ARG	NE-CZ-NH2	-16.98	111.81	120.30
1	B	381	ARG	NE-CZ-NH2	-16.20	112.20	120.30
1	A	381	ARG	NE-CZ-NH2	-15.80	112.40	120.30
1	A	289	ARG	NE-CZ-NH1	15.73	128.17	120.30
1	B	68	GLU	CA-CB-CG	15.22	146.88	113.40
1	A	30	ARG	NE-CZ-NH2	-14.38	113.11	120.30
1	B	108	ARG	NE-CZ-NH2	-13.88	113.36	120.30
1	B	381	ARG	NE-CZ-NH1	13.27	126.94	120.30
1	B	187	ARG	NE-CZ-NH2	-13.26	113.67	120.30
1	B	299	ASP	CB-CG-OD1	12.44	129.49	118.30
1	A	156	ARG	NE-CZ-NH2	-12.07	114.27	120.30
1	B	98	PHE	CB-CG-CD2	-11.88	112.48	120.80
1	A	249	ARG	CD-NE-CZ	11.81	140.13	123.60
1	B	394	ARG	NE-CZ-NH2	-11.41	114.59	120.30
1	A	299	ASP	CB-CG-OD1	11.08	128.27	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	PHE	CB-CG-CD2	-11.03	113.08	120.80
1	B	111	ARG	NE-CZ-NH1	10.99	125.80	120.30
1	A	149	ASP	CB-CG-OD1	10.85	128.07	118.30
1	A	241	PHE	CB-CG-CD1	10.75	128.32	120.80
1	B	68	GLU	CB-CG-CD	10.63	142.91	114.20
1	B	244	ASP	CB-CG-OD1	10.61	127.85	118.30
1	B	379	PHE	CB-CG-CD1	-10.44	113.49	120.80
1	A	315	TYR	CB-CG-CD1	10.42	127.25	121.00
1	A	297	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	A	23	ASP	CB-CG-OD1	10.35	127.61	118.30
1	B	30	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	B	213	LEU	CA-CB-CG	10.05	138.41	115.30
1	A	249	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	B	98	PHE	CB-CG-CD1	9.88	127.72	120.80
1	A	158	ARG	CD-NE-CZ	9.71	137.19	123.60
1	B	149	ASP	CB-CG-OD1	9.69	127.02	118.30
1	A	375	ARG	NE-CZ-NH2	-9.60	115.50	120.30
1	A	144	TYR	CB-CG-CD1	-9.52	115.29	121.00
1	A	381	ARG	CD-NE-CZ	9.31	136.64	123.60
1	B	93	PHE	CB-CG-CD1	-9.19	114.37	120.80
1	A	12	PHE	CB-CG-CD2	9.06	127.14	120.80
1	A	30	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	B	111	ARG	NE-CZ-NH2	-8.99	115.81	120.30
1	B	370	GLU	OE1-CD-OE2	8.93	134.01	123.30
1	A	103	PHE	CB-CG-CD1	8.84	126.99	120.80
1	A	289	ARG	CD-NE-CZ	8.79	135.90	123.60
1	A	111	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	315	TYR	CB-CG-CD2	-8.64	115.81	121.00
1	A	379	PHE	CB-CG-CD2	-8.62	114.77	120.80
1	B	374	GLU	CA-CB-CG	8.62	132.36	113.40
1	A	139	ARG	NE-CZ-NH2	8.61	124.60	120.30
1	A	241	PHE	CB-CG-CD2	-8.59	114.79	120.80
1	B	30	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	A	254	ASP	CB-CG-OD2	-8.47	110.68	118.30
1	A	189	ASP	CB-CG-OD1	-8.44	110.70	118.30
1	A	44	GLU	CA-CB-CG	8.24	131.53	113.40
1	A	326	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	B	111	ARG	CD-NE-CZ	8.10	134.94	123.60
1	A	297	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	A	103	PHE	CB-CG-CD2	-8.09	115.14	120.80
1	A	113	PHE	CB-CG-CD2	-8.05	115.16	120.80
1	B	23	ASP	CB-CA-C	8.02	126.44	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	TYR	CB-CG-CD2	-7.97	116.22	121.00
1	B	167	TYR	CB-CG-CD1	7.95	125.77	121.00
1	B	144	TYR	CB-CG-CD1	-7.94	116.23	121.00
1	B	139	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	B	174	ASN	N-CA-CB	7.74	124.54	110.60
1	A	379	PHE	CB-CG-CD1	7.68	126.17	120.80
1	B	272	ASP	CB-CG-OD2	7.59	125.13	118.30
1	A	43	ALA	CB-CA-C	7.52	121.38	110.10
1	B	156	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	A	12	PHE	CB-CG-CD1	-7.51	115.54	120.80
1	B	144	TYR	CB-CG-CD2	7.50	125.50	121.00
1	B	259	PHE	CB-CG-CD1	7.49	126.04	120.80
1	A	6	PRO	C-N-CA	7.46	140.36	121.70
1	A	112	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	223	ALA	N-CA-CB	7.43	120.50	110.10
1	A	301	TYR	CB-CG-CD2	-7.39	116.56	121.00
1	B	53	HIS	N-CA-CB	7.39	123.91	110.60
1	B	254	ASP	CB-CG-OD1	7.37	124.93	118.30
1	B	229	HIS	CA-C-N	7.33	130.86	116.20
1	B	321	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	187	ARG	CA-CB-CG	7.28	129.42	113.40
1	A	144	TYR	CB-CG-CD2	7.23	125.34	121.00
1	A	269	PHE	CB-CG-CD2	-7.19	115.77	120.80
1	B	263	ASP	CB-CG-OD2	7.18	124.77	118.30
1	A	61	ASP	CB-CG-OD2	7.16	124.75	118.30
1	B	23	ASP	CB-CG-OD2	7.15	124.74	118.30
1	B	358	MET	C-N-CA	7.14	139.56	121.70
1	B	93	PHE	CB-CG-CD2	7.14	125.80	120.80
1	A	189	ASP	CB-CG-OD2	7.11	124.70	118.30
1	B	105	SER	N-CA-CB	7.06	121.09	110.50
1	A	289	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	194	THR	CA-CB-CG2	7.01	122.21	112.40
1	A	309	LYS	CA-CB-CG	6.98	128.76	113.40
1	B	382	LEU	CB-CG-CD1	6.98	122.86	111.00
1	B	193	PRO	O-C-N	-6.96	111.56	122.70
1	B	203	GLU	OE1-CD-OE2	-6.92	115.00	123.30
1	B	203	GLU	CG-CD-OE2	6.88	132.06	118.30
1	B	384	GLN	CG-CD-OE1	6.82	135.23	121.60
1	B	98	PHE	CG-CD2-CE2	6.79	128.27	120.80
1	A	103	PHE	CA-CB-CG	6.76	130.13	113.90
1	B	253	TYR	CB-CG-CD2	-6.74	116.96	121.00
1	B	253	TYR	CB-CG-CD1	6.72	125.03	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	GLU	CA-CB-CG	6.71	128.16	113.40
1	A	360	ASP	CB-CG-OD1	6.66	124.30	118.30
1	A	68	GLU	CB-CG-CD	6.66	132.17	114.20
1	A	180	GLU	CA-CB-CG	6.64	128.00	113.40
1	B	342	GLU	CG-CD-OE2	-6.57	105.15	118.30
1	A	143	GLU	OE1-CD-OE2	-6.52	115.48	123.30
1	B	195	VAL	CA-C-N	6.50	129.21	116.20
1	B	217	THR	C-N-CA	6.49	135.92	122.30
1	B	263	ASP	OD1-CG-OD2	-6.48	111.00	123.30
1	B	187	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	B	263	ASP	CB-CG-OD1	6.46	124.11	118.30
1	B	289	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	B	220	GLU	C-N-CA	6.42	137.74	121.70
1	B	273	LEU	CA-CB-CG	6.39	129.99	115.30
1	A	328	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	67	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	22	ALA	CB-CA-C	6.38	119.67	110.10
1	A	190	ILE	O-C-N	6.26	132.72	122.70
1	B	115	LEU	CB-CA-C	6.24	122.06	110.20
1	B	279	PRO	C-N-CA	6.23	137.28	121.70
1	A	111	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	B	156	ARG	NH1-CZ-NH2	-6.15	112.64	119.40
1	B	104	THR	C-N-CA	6.14	137.06	121.70
1	B	44	GLU	CA-CB-CG	6.14	126.91	113.40
1	B	83	LEU	CA-CB-CG	6.13	129.40	115.30
1	A	254	ASP	CA-CB-CG	6.12	126.87	113.40
1	A	305	TRP	CB-CA-C	6.10	122.60	110.40
1	A	301	TYR	CB-CG-CD1	6.10	124.66	121.00
1	A	316	LEU	CB-CA-C	6.10	121.79	110.20
1	A	392	GLY	C-N-CA	6.10	136.94	121.70
1	B	263	ASP	CB-CA-C	6.09	122.59	110.40
1	B	143	GLU	N-CA-CB	6.09	121.57	110.60
1	B	383	ASN	CB-CG-OD1	-6.08	109.43	121.60
1	B	286	THR	CA-CB-OG1	-6.08	96.24	109.00
1	A	320	GLU	OE1-CD-OE2	-6.07	116.01	123.30
1	B	148	LYS	CB-CA-C	-6.07	98.26	110.40
1	A	225	LEU	CB-CA-C	6.06	121.72	110.20
1	B	113	PHE	CB-CG-CD2	-6.04	116.57	120.80
1	B	372	ALA	O-C-N	-6.04	113.03	122.70
1	B	108	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	224	GLY	CA-C-O	-6.04	109.73	120.60
1	B	375	ARG	NE-CZ-NH1	6.03	123.31	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	289	ARG	CD-NE-CZ	6.01	132.02	123.60
1	A	209	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	145	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	150	LEU	CB-CA-C	5.97	121.55	110.20
1	B	107	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	B	127	GLU	CA-CB-CG	5.95	126.50	113.40
1	A	259	PHE	C-N-CA	5.92	134.72	122.30
1	B	297	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	B	98	PHE	CZ-CE2-CD2	-5.91	113.01	120.10
1	A	2	VAL	CB-CA-C	5.91	122.62	111.40
1	B	286	THR	CA-CB-CG2	5.91	120.67	112.40
1	A	249	ARG	CB-CA-C	5.90	122.20	110.40
1	A	333	GLU	OE1-CD-OE2	5.87	130.34	123.30
1	B	188	GLY	O-C-N	-5.86	113.33	122.70
1	B	118	VAL	CA-CB-CG2	-5.86	102.12	110.90
1	A	196	GLY	C-N-CA	5.84	136.31	121.70
1	B	377	PHE	CB-CG-CD1	-5.84	116.71	120.80
1	A	96	PRO	O-C-N	-5.83	113.37	122.70
1	A	333	GLU	CG-CD-OE1	-5.83	106.65	118.30
1	B	68	GLU	N-CA-CB	5.82	121.08	110.60
1	A	252	LYS	CD-CE-NZ	5.82	125.08	111.70
1	A	215	PRO	O-C-N	5.81	132.00	122.70
1	A	227	PHE	N-CA-CB	5.81	121.06	110.60
1	A	305	TRP	O-C-N	-5.79	113.43	122.70
1	A	30	ARG	CD-NE-CZ	5.79	131.70	123.60
1	B	106	ASN	N-CA-CB	5.78	121.01	110.60
1	A	72	GLY	O-C-N	-5.73	113.53	122.70
1	B	320	GLU	N-CA-CB	5.73	120.92	110.60
1	B	156	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	111	ARG	CG-CD-NE	5.72	123.82	111.80
1	A	213	LEU	CA-CB-CG	5.68	128.37	115.30
1	B	368	ASP	CB-CG-OD1	5.67	123.41	118.30
1	B	208	GLY	C-N-CA	5.65	135.83	121.70
1	A	135	MET	CG-SD-CE	5.65	109.24	100.20
1	A	80	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	254	ASP	N-CA-CB	5.63	120.73	110.60
1	A	320	GLU	CG-CD-OE2	5.62	129.55	118.30
1	A	211	VAL	CA-CB-CG2	5.62	119.33	110.90
1	B	244	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	139	ARG	NH1-CZ-NH2	-5.58	113.26	119.40
1	A	375	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	299	ASP	CB-CG-OD2	-5.57	113.29	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	PRO	CA-C-N	5.55	129.40	117.20
1	B	324	ALA	N-CA-CB	-5.54	102.34	110.10
1	A	174	ASN	CB-CA-C	5.54	121.47	110.40
1	A	285	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	B	193	PRO	CA-C-N	5.53	129.37	117.20
1	B	249	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	44	GLU	CG-CD-OE1	-5.50	107.30	118.30
1	A	149	ASP	N-CA-CB	5.49	120.48	110.60
1	A	179	LEU	CA-CB-CG	5.49	127.92	115.30
1	B	342	GLU	CG-CD-OE1	5.48	129.25	118.30
1	A	53	HIS	N-CA-CB	5.47	120.45	110.60
1	B	254	ASP	CB-CA-C	5.45	121.30	110.40
1	A	370	GLU	CA-CB-CG	5.44	125.37	113.40
1	B	223	ALA	C-N-CA	5.43	133.69	122.30
1	A	136	TRP	N-CA-CB	5.42	120.36	110.60
1	A	393	SER	CB-CA-C	-5.42	99.81	110.10
1	B	175	LEU	O-C-N	5.42	131.37	122.70
1	B	220	GLU	CG-CD-OE2	-5.41	107.48	118.30
1	B	149	ASP	N-CA-C	-5.40	96.43	111.00
1	B	223	ALA	O-C-N	-5.39	114.03	123.20
1	A	83	LEU	CA-CB-CG	5.38	127.69	115.30
1	B	220	GLU	CG-CD-OE1	5.38	129.05	118.30
1	B	328	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	299	ASP	OD1-CG-OD2	-5.34	113.16	123.30
1	B	43	ALA	C-N-CA	5.31	134.98	121.70
1	B	343	LEU	C-N-CA	5.31	133.45	122.30
1	A	96	PRO	CA-C-N	5.31	128.87	117.20
1	B	257	LEU	O-C-N	5.30	131.18	122.70
1	A	187	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	B	247	GLY	CA-C-O	5.29	130.13	120.60
1	A	12	PHE	CG-CD1-CE1	5.29	126.62	120.80
1	A	51	THR	CA-CB-CG2	5.28	119.79	112.40
1	B	360	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	278	PHE	CB-CG-CD1	-5.26	117.12	120.80
1	B	195	VAL	CA-C-O	-5.26	109.06	120.10
1	A	73	ASP	N-CA-CB	5.25	120.05	110.60
1	A	341	PHE	CB-CG-CD1	-5.25	117.13	120.80
1	A	273	LEU	CA-CB-CG	5.23	127.34	115.30
1	A	379	PHE	CA-CB-CG	5.23	126.45	113.90
1	B	359	ASN	N-CA-CB	-5.22	101.20	110.60
1	B	229	HIS	CA-C-O	-5.21	109.16	120.10
1	A	145	ASP	CA-C-N	5.20	126.60	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	THR	C-N-CA	5.20	134.70	121.70
1	A	113	PHE	CB-CG-CD1	5.18	124.43	120.80
1	A	289	ARG	N-CA-CB	5.17	119.90	110.60
1	A	68	GLU	OE1-CD-OE2	-5.17	117.10	123.30
1	B	113	PHE	CB-CG-CD1	5.16	124.41	120.80
1	B	5	THR	N-CA-CB	5.16	120.11	110.30
1	B	119	LEU	CB-CA-C	5.16	120.01	110.20
1	A	270	THR	CA-CB-CG2	5.16	119.62	112.40
1	B	97	VAL	CA-CB-CG1	5.15	118.63	110.90
1	A	257	LEU	CA-CB-CG	5.15	127.15	115.30
1	B	7	ALA	N-CA-CB	5.14	117.30	110.10
1	B	56	ASP	N-CA-CB	5.13	119.83	110.60
1	B	238	GLU	CB-CG-CD	5.13	128.05	114.20
1	B	189	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	174	ASN	CB-CG-OD1	-5.11	111.38	121.60
1	B	340	VAL	CB-CA-C	5.11	121.11	111.40
1	A	149	ASP	N-CA-C	-5.11	97.21	111.00
1	B	383	ASN	CB-CG-ND2	5.11	128.96	116.70
1	A	308	ALA	N-CA-CB	5.09	117.23	110.10
1	A	249	ARG	O-C-N	-5.09	114.55	123.20
1	A	267	ALA	CB-CA-C	5.07	117.71	110.10
1	A	216	GLU	OE1-CD-OE2	5.07	129.38	123.30
1	A	52	PHE	CB-CG-CD2	-5.06	117.26	120.80
1	B	5	THR	CA-CB-CG2	5.05	119.47	112.40
1	B	272	ASP	CB-CG-OD1	-5.03	113.77	118.30
1	B	391	LEU	C-N-CA	5.03	132.87	122.30
1	A	96	PRO	C-N-CA	5.02	134.26	121.70
1	A	238	GLU	CG-CD-OE2	-5.01	108.28	118.30
1	A	314	MET	N-CA-CB	5.01	119.62	110.60

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	3026	0	2888	24	0
1	B	3026	0	2886	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	298	0	0	3	0
3	B	288	0	0	1	1
All	All	6640	0	5774	45	1

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:A:95:HIS:HD2	1:A:97:VAL:H	1.36	0.73
1:B:184:ASN:HA	1:B:190:ILE:HG13	1.77	0.66
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.79	0.63
1:B:95:HIS:HD2	1:B:97:VAL:H	1.46	0.63
1:B:148:LYS:HG3	1:B:191:PHE:HZ	1.69	0.57
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.87	0.56
1:B:182:LYS:HE2	1:B:184:ASN:O	2.07	0.56
1:A:215:PRO:HG2	1:A:231:ILE:HG22	1.88	0.55
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.88	0.55
1:A:249:ARG:O	1:A:252:LYS:HE3	2.08	0.53
1:B:319:LYS:O	1:B:323:LEU:HG	2.09	0.53
1:A:2:VAL:HG13	1:A:316:LEU:HB2	1.90	0.51
1:B:235:LEU:HD12	1:B:273:LEU:HD11	1.93	0.51
1:A:299:ASP:HB3	1:A:303:GLY:HA3	1.93	0.50
1:A:195:VAL:HG22	1:A:213:LEU:HD12	1.93	0.50
1:B:35:PRO:O	1:B:39:VAL:HG23	2.11	0.49
1:B:55:ASN:HA	1:B:58:ILE:O	2.13	0.49
1:A:58:ILE:HD11	1:A:71:LEU:HD21	1.93	0.49
1:B:43:ALA:HA	1:B:83:LEU:HD21	1.94	0.48
1:A:273:LEU:HD23	3:A:584(A):HOH:O	2.15	0.47
1:A:363:SER:HB2	3:A:619(A):HOH:O	2.14	0.47
1:A:328:ASP:HA	1:A:329:PRO:HD3	1.74	0.46
1:A:289:ARG:HD3	3:A:404(A):HOH:O	2.15	0.46
1:B:182:LYS:HA	1:B:183:PRO:HD3	1.74	0.46
1:A:216:GLU:HB2	1:A:244:ASP:HB2	1.98	0.45
1:A:55:ASN:HA	1:A:58:ILE:O	2.16	0.45
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.97	0.45
1:A:95:HIS:CD2	1:A:97:VAL:H	2.25	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.82	0.44
1:B:328:ASP:HA	1:B:329:PRO:HD3	1.78	0.44
1:B:275:GLU:OE1	1:B:319:LYS:HE3	2.17	0.43
1:A:261:HIS:NE2	1:B:384:GLN:NE2	2.67	0.43
1:B:294:LYS:HA	1:B:295:PRO:HD3	1.85	0.43
1:B:179:LEU:O	1:B:181:PRO:HD3	2.19	0.42
1:B:273:LEU:O	1:B:273:LEU:HD12	2.19	0.42
1:A:185:GLU:HA	1:A:186:PRO:HA	1.73	0.42
1:B:208:GLY:HA3	3:B:572(B):HOH:O	2.19	0.42
1:B:278:PHE:HA	1:B:279:PRO:HD3	1.91	0.41
1:A:192:LEU:N	1:A:193:PRO:CD	2.83	0.41
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.55	0.41
1:A:122:ILE:HG23	1:A:175:LEU:HD12	2.02	0.41
1:A:217:THR:HA	1:A:227:PHE:CD1	2.56	0.41
1:A:51:THR:CG2	1:A:87:MET:HB3	2.51	0.40
1:A:235:LEU:HG	1:A:240:LEU:HD23	2.03	0.40
1:B:235:LEU:HD22	1:B:283:PRO:HB2	2.04	0.40

All (1) 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)
3:B:573(B):HOH:O	3:B:614(B):HOH:O[4_555]	2.15	0.05

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%)	375 (96%)	15 (4%)	1 (0%)	41	61
1	B	391/394 (99%)	379 (97%)	10 (3%)	2 (0%)	29	48
All	All	782/788 (99%)	754 (96%)	25 (3%)	3 (0%)	34	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU
1	B	185	GLU
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%)	293 (96%)	12 (4%)	32	57
1	B	305/310 (98%)	295 (97%)	10 (3%)	38	64
All	All	610/620 (98%)	588 (96%)	22 (4%)	35	61

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	GLU
1	A	90	THR
1	A	94	SER
1	A	149	ASP
1	A	184	ASN
1	A	213	LEU
1	A	273	LEU
1	A	289	ARG
1	A	313	SER
1	A	333	GLU
1	A	361	SER
1	A	393	SER
1	B	34	ASP
1	B	41	LYS
1	B	68	GLU
1	B	174	ASN
1	B	193	PRO
1	B	235	LEU
1	B	273	LEU
1	B	320	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	333	GLU
1	B	393	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) 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	9	HIS
1	B	75	ASN
1	B	95	HIS
1	B	384	GLN

5.3.3 RNA [i](#)

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 2 ligands modelled in this entry, 2 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.