



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:30 PM GMT

PDB ID : 1XLA
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 : 2.30 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

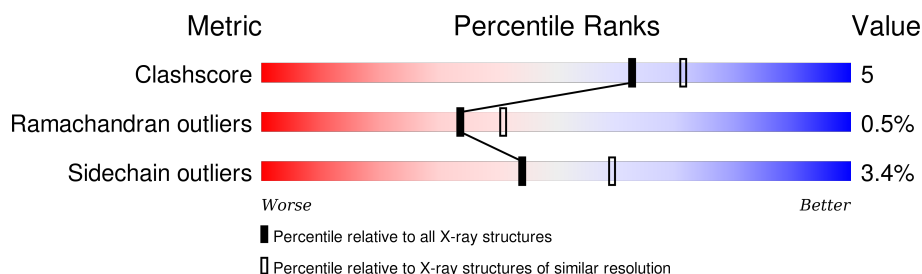
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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	
1	B	394	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6631 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 water.

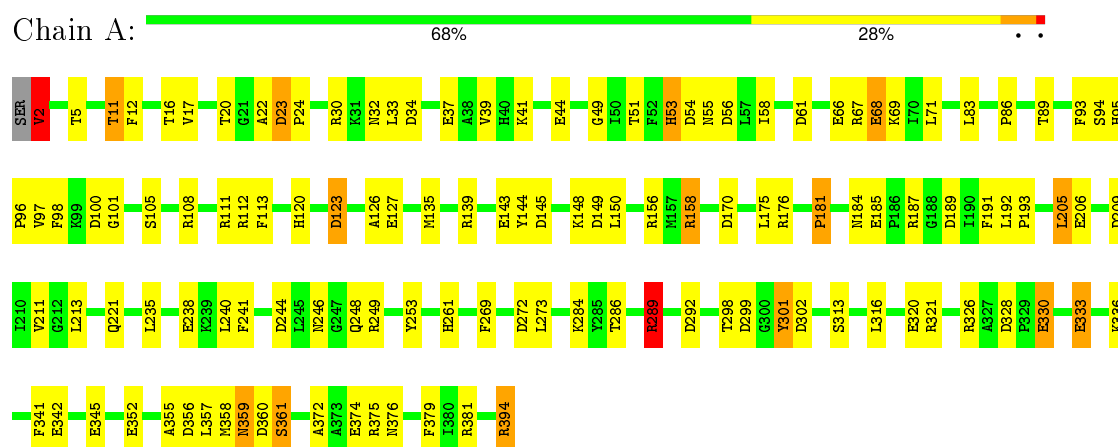
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	292	Total	O	0	0
			292	292		
2	B	287	Total	O	0	0
			287	287		

3 Residue-property plots

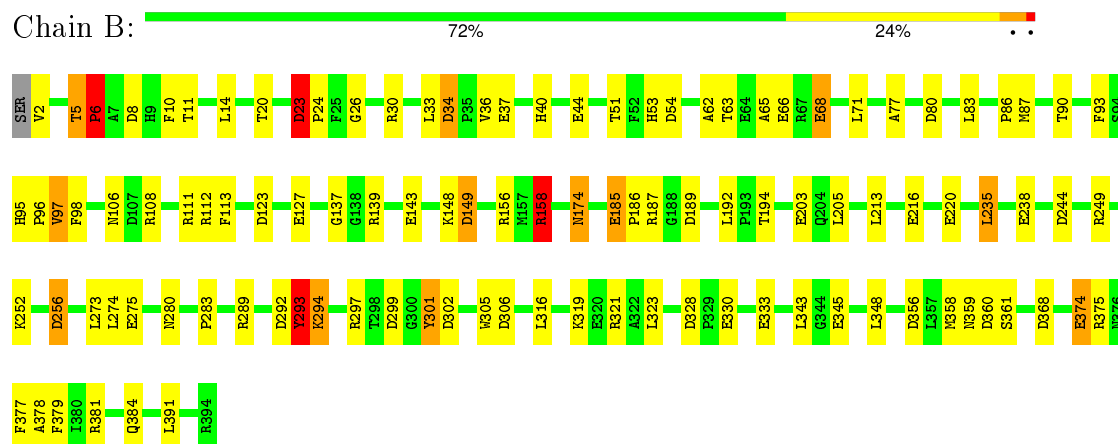
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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	105.70 Å 105.70 Å 154.10 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6631	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.15	3/3100 (0.1%)	2.19	123/4201 (2.9%)
1	B	1.12	1/3100 (0.0%)	2.04	104/4201 (2.5%)
All	All	1.13	4/6200 (0.1%)	2.11	227/8402 (2.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	ASP	CA-C	-10.66	1.25	1.52
1	A	302	ASP	N-CA	8.67	1.63	1.46
1	A	158	ARG	CD-NE	-7.66	1.33	1.46
1	B	220	GLU	CD-OE1	-5.46	1.19	1.25

All (227) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	289	ARG	CD-NE-CZ	27.09	161.52	123.60
1	A	158	ARG	CD-NE-CZ	20.10	151.74	123.60
1	A	289	ARG	NE-CZ-NH2	-19.36	110.62	120.30
1	A	158	ARG	NE-CZ-NH2	-19.14	110.73	120.30
1	A	158	ARG	NE-CZ-NH1	18.81	129.71	120.30
1	B	189	ASP	CB-CG-OD2	17.88	134.39	118.30
1	A	289	ARG	NE-CZ-NH1	16.48	128.54	120.30
1	A	111	ARG	NE-CZ-NH1	16.43	128.51	120.30
1	A	375	ARG	NE-CZ-NH1	14.41	127.50	120.30
1	B	297	ARG	NE-CZ-NH2	13.06	126.83	120.30
1	A	301	TYR	CB-CG-CD1	-12.94	113.24	121.00
1	A	249	ARG	NE-CZ-NH1	12.84	126.72	120.30
1	A	375	ARG	NE-CZ-NH2	-12.58	114.01	120.30
1	A	333	GLU	N-CA-CB	-12.54	88.03	110.60
1	B	30	ARG	NE-CZ-NH1	12.51	126.55	120.30
1	A	381	ARG	NE-CZ-NH2	-12.19	114.21	120.30
1	B	71	LEU	N-CA-CB	12.10	134.59	110.40
1	A	326	ARG	NE-CZ-NH2	-11.84	114.38	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ARG	NE-CZ-NH2	-11.77	114.42	120.30
1	A	170	ASP	CB-CG-OD2	-11.75	107.73	118.30
1	B	381	ARG	NE-CZ-NH2	-11.69	114.45	120.30
1	A	345	GLU	OE1-CD-OE2	-11.63	109.34	123.30
1	B	112	ARG	CD-NE-CZ	11.40	139.56	123.60
1	B	44	GLU	CA-CB-CG	11.34	138.34	113.40
1	B	299	ASP	CB-CG-OD1	11.03	128.23	118.30
1	A	209	ASP	CB-CG-OD1	10.91	128.12	118.30
1	A	113	PHE	CB-CG-CD2	-10.90	113.17	120.80
1	A	61	ASP	CB-CG-OD2	10.83	128.05	118.30
1	B	71	LEU	CB-CA-C	-10.72	89.83	110.20
1	A	156	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	A	108	ARG	NE-CZ-NH1	10.55	125.58	120.30
1	A	2	VAL	O-C-N	-10.45	105.97	122.70
1	A	112	ARG	CD-NE-CZ	10.45	138.23	123.60
1	B	149	ASP	CB-CG-OD1	10.43	127.68	118.30
1	B	244	ASP	CB-CG-OD1	10.41	127.67	118.30
1	B	374	GLU	OE1-CD-OE2	-10.09	111.19	123.30
1	A	272	ASP	CB-CG-OD2	10.08	127.37	118.30
1	B	34	ASP	CB-CG-OD1	9.86	127.17	118.30
1	A	158	ARG	CG-CD-NE	9.84	132.46	111.80
1	B	358	MET	C-N-CA	9.78	146.15	121.70
1	A	358	MET	C-N-CA	9.77	146.11	121.70
1	A	187	ARG	NE-CZ-NH2	-9.49	115.56	120.30
1	A	67	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	B	123	ASP	CB-CG-OD2	9.36	126.72	118.30
1	B	111	ARG	NE-CZ-NH1	9.33	124.96	120.30
1	A	326	ARG	NE-CZ-NH1	9.29	124.95	120.30
1	A	299	ASP	CB-CG-OD1	9.11	126.49	118.30
1	B	273	LEU	CA-CB-CG	9.01	136.01	115.30
1	A	139	ARG	NE-CZ-NH2	8.99	124.80	120.30
1	A	302	ASP	CB-CA-C	8.85	128.10	110.40
1	A	333	GLU	CB-CG-CD	8.75	137.82	114.20
1	A	20	THR	N-CA-CB	8.63	126.70	110.30
1	A	241	PHE	CB-CG-CD1	8.60	126.82	120.80
1	B	189	ASP	CB-CG-OD1	-8.55	110.61	118.30
1	B	289	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	B	139	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	B	23	ASP	CB-CA-C	8.22	126.85	110.40
1	A	111	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	A	112	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	A	302	ASP	CB-CG-OD1	-8.12	110.99	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	ARG	CD-NE-CZ	8.10	134.93	123.60
1	A	302	ASP	CB-CG-OD2	8.06	125.55	118.30
1	A	145	ASP	CB-CG-OD1	-7.93	111.16	118.30
1	B	203	GLU	OE1-CD-OE2	-7.92	113.80	123.30
1	A	342	GLU	OE1-CD-OE2	7.84	132.70	123.30
1	A	54	ASP	CB-CG-OD2	7.79	125.31	118.30
1	A	356	ASP	CB-CG-OD2	7.79	125.31	118.30
1	A	342	GLU	CG-CD-OE2	-7.77	102.76	118.30
1	B	158	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	113	PHE	CB-CG-CD1	7.75	126.22	120.80
1	B	108	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	381	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	B	328	ASP	CB-CG-OD1	7.57	125.11	118.30
1	A	301	TYR	CB-CG-CD2	7.56	125.54	121.00
1	B	93	PHE	CB-CG-CD1	7.51	126.05	120.80
1	A	67	ARG	CD-NE-CZ	7.50	134.10	123.60
1	A	249	ARG	CD-NE-CZ	7.48	134.08	123.60
1	B	97	VAL	CA-CB-CG1	7.44	122.06	110.90
1	A	112	ARG	CG-CD-NE	-7.43	96.20	111.80
1	B	203	GLU	CG-CD-OE2	7.25	132.81	118.30
1	A	238	GLU	OE1-CD-OE2	7.22	131.97	123.30
1	A	23	ASP	CB-CG-OD1	7.21	124.79	118.30
1	B	113	PHE	CB-CG-CD2	-7.17	115.78	120.80
1	A	108	ARG	CD-NE-CZ	7.14	133.60	123.60
1	A	170	ASP	CB-CG-OD1	7.08	124.68	118.30
1	B	321	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	194	THR	CA-CB-CG2	7.01	122.22	112.40
1	A	150	LEU	CB-CA-C	6.97	123.44	110.20
1	B	375	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	139	ARG	NH1-CZ-NH2	-6.95	111.76	119.40
1	A	272	ASP	CB-CG-OD1	-6.95	112.05	118.30
1	B	299	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	A	12	PHE	CB-CG-CD1	-6.91	115.96	120.80
1	B	156	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	34	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	374	GLU	OE1-CD-OE2	6.86	131.53	123.30
1	A	44	GLU	CA-CB-CG	6.84	128.45	113.40
1	A	360	ASP	CB-CG-OD2	6.79	124.42	118.30
1	B	143	GLU	OE1-CD-OE2	-6.76	115.19	123.30
1	A	253	TYR	CB-CG-CD1	6.76	125.06	121.00
1	B	112	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	158	ARG	NE-CZ-NH1	6.75	123.68	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	368	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	176	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	174	ASN	CB-CA-C	6.60	123.59	110.40
1	B	6	PRO	CA-C-N	6.59	131.69	117.20
1	A	211	VAL	CA-CB-CG2	6.58	120.76	110.90
1	B	148	LYS	CD-CE-NZ	6.57	126.81	111.70
1	B	54	ASP	O-C-N	-6.53	112.25	122.70
1	B	8	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	206	GLU	OE1-CD-OE2	-6.51	115.49	123.30
1	B	80	ASP	CB-CG-OD1	6.51	124.16	118.30
1	B	356	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	20	THR	CA-CB-CG2	6.38	121.33	112.40
1	B	112	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	80	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	B	14	LEU	CB-CA-C	6.35	122.26	110.20
1	A	144	TYR	CB-CG-CD1	-6.34	117.20	121.00
1	B	391	LEU	C-N-CA	6.33	135.60	122.30
1	A	320	GLU	CA-CB-CG	6.31	127.29	113.40
1	A	139	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	394	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	44	GLU	CB-CA-C	-6.28	97.84	110.40
1	B	158	ARG	CD-NE-CZ	6.24	132.34	123.60
1	B	23	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	345	GLU	CG-CD-OE2	6.18	130.66	118.30
1	A	244	ASP	CB-CG-OD1	6.13	123.81	118.30
1	A	156	ARG	NH1-CZ-NH2	-6.09	112.70	119.40
1	B	192	LEU	CA-CB-CG	6.09	129.32	115.30
1	B	359	ASN	N-CA-CB	-6.08	99.65	110.60
1	A	175	LEU	CB-CA-C	-6.04	98.72	110.20
1	A	372	ALA	C-N-CA	6.04	136.79	121.70
1	B	216	GLU	CG-CD-OE1	6.01	130.32	118.30
1	A	22	ALA	CB-CA-C	5.98	119.06	110.10
1	B	379	PHE	CB-CG-CD1	5.98	124.98	120.80
1	A	241	PHE	CB-CG-CD2	-5.96	116.62	120.80
1	B	137	GLY	C-N-CA	5.96	134.82	122.30
1	B	30	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	394	ARG	CA-CB-CG	5.92	126.42	113.40
1	B	37	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	B	297	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	B	333	GLU	CG-CD-OE1	-5.85	106.60	118.30
1	B	127	GLU	CG-CD-OE2	5.85	130.00	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	ARG	NH1-CZ-NH2	-5.83	112.98	119.40
1	B	113	PHE	CB-CG-CD1	5.83	124.88	120.80
1	B	348	LEU	CA-CB-CG	5.81	128.66	115.30
1	B	280	ASN	CA-C-N	5.80	127.80	116.20
1	B	10	PHE	CB-CG-CD1	5.75	124.82	120.80
1	B	345	GLU	CG-CD-OE2	5.74	129.78	118.30
1	A	143	GLU	OE1-CD-OE2	-5.73	116.42	123.30
1	A	149	ASP	N-CA-C	-5.73	95.53	111.00
1	B	40	HIS	CA-CB-CG	-5.73	103.86	113.60
1	A	145	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	100	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	292	ASP	C-N-CA	5.68	135.91	121.70
1	A	321	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	B	216	GLU	CG-CD-OE2	-5.66	106.99	118.30
1	A	53	HIS	N-CA-CB	5.61	120.70	110.60
1	B	53	HIS	N-CA-CB	5.61	120.70	110.60
1	A	209	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	B	93	PHE	CB-CG-CD2	-5.60	116.88	120.80
1	B	97	VAL	CG1-CB-CG2	-5.59	101.95	110.90
1	B	83	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	30	ARG	CD-NE-CZ	5.54	131.36	123.60
1	A	379	PHE	CA-CB-CG	5.53	127.17	113.90
1	A	352	GLU	CG-CD-OE2	5.48	129.26	118.30
1	B	51	THR	CA-CB-CG2	5.48	120.07	112.40
1	A	249	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	98	PHE	CB-CG-CD2	-5.47	116.97	120.80
1	A	206	GLU	CA-CB-CG	5.46	125.42	113.40
1	A	372	ALA	O-C-N	-5.46	113.97	122.70
1	A	286	THR	N-CA-CB	5.45	120.65	110.30
1	A	328	ASP	CB-CG-OD1	5.45	123.20	118.30
1	B	305	TRP	CB-CA-C	5.45	121.29	110.40
1	A	292	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	298	THR	C-N-CA	5.44	135.30	121.70
1	A	11	THR	CA-CB-CG2	5.43	120.01	112.40
1	A	376	ASN	N-CA-CB	5.42	120.36	110.60
1	B	293	TYR	CB-CG-CD2	-5.41	117.76	121.00
1	A	105	SER	C-N-CA	5.40	135.20	121.70
1	A	41	LYS	N-CA-CB	5.39	120.31	110.60
1	B	187	ARG	CD-NE-CZ	5.38	131.14	123.60
1	A	56	ASP	N-CA-CB	5.38	120.29	110.60
1	B	330	GLU	CG-CD-OE1	-5.38	107.55	118.30
1	A	123	ASP	CB-CG-OD1	5.38	123.14	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	GLY	O-C-N	5.36	132.31	123.20
1	A	189	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	B	5	THR	N-CA-CB	5.35	120.46	110.30
1	B	149	ASP	N-CA-C	-5.35	96.57	111.00
1	A	53	HIS	CB-CA-C	-5.34	99.72	110.40
1	A	302	ASP	N-CA-CB	-5.33	101.00	110.60
1	A	67	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	269	PHE	CB-CG-CD1	-5.31	117.08	120.80
1	B	108	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	127	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	B	360	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	341	PHE	CB-CG-CD1	-5.29	117.10	120.80
1	A	205	LEU	CA-CB-CG	5.28	127.43	115.30
1	B	375	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	213	LEU	CA-CB-CG	5.26	127.39	115.30
1	B	301	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	A	246	ASN	N-CA-CB	5.24	120.03	110.60
1	A	126	ALA	CB-CA-C	5.21	117.91	110.10
1	A	20	THR	CA-CB-CG2	5.20	119.68	112.40
1	B	274	LEU	CB-CG-CD1	-5.20	102.16	111.00
1	B	10	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	B	379	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	B	294	LYS	CB-CA-C	-5.16	100.09	110.40
1	B	87	MET	CG-SD-CE	5.13	108.42	100.20
1	B	238	GLU	CA-CB-CG	5.13	124.69	113.40
1	A	51	THR	CA-CB-CG2	5.13	119.58	112.40
1	A	144	TYR	CA-C-O	5.11	130.84	120.10
1	B	26	GLY	CA-C-O	5.11	129.80	120.60
1	A	135	MET	CG-SD-CE	5.09	108.34	100.20
1	B	96	PRO	CA-C-N	5.09	128.40	117.20
1	A	93	PHE	CB-CG-CD1	-5.09	117.24	120.80
1	B	98	PHE	CB-CG-CD2	-5.09	117.24	120.80
1	A	96	PRO	O-C-N	-5.06	114.60	122.70
1	B	187	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	66	GLU	CG-CD-OE2	5.03	128.36	118.30
1	A	357	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	B	256	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	B	34	ASP	OD1-CG-OD2	-5.01	113.78	123.30
1	B	106	ASN	C-N-CA	5.01	134.22	121.70
1	B	306	ASP	CB-CG-OD2	5.01	122.81	118.30
1	B	302	ASP	C-N-CA	5.00	132.81	122.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3026	0	2886	41	0
1	B	3026	0	2887	23	3
2	A	292	0	0	14	0
2	B	287	0	0	2	2
All	All	6631	0	5773	63	3

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 (63) 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:2:VAL:HG22	1:A:316:LEU:HB2	1.40	1.01
1:A:2:VAL:HG22	1:A:316:LEU:CB	1.93	0.99
1:A:68:GLU:HG2	2:A:592(A):HOH:O	1.65	0.95
1:B:33:LEU:HB2	1:B:301:TYR:OH	1.68	0.93
1:A:333:GLU:OE2	2:A:642(A):HOH:O	1.89	0.90
1:A:68:GLU:OE2	2:A:597(A):HOH:O	1.95	0.85
1:B:256:ASP:HB3	1:B:293:TYR:HA	1.62	0.81
1:B:95:HIS:HD2	1:B:97:VAL:H	1.32	0.78
1:B:2:VAL:O	1:B:2:VAL:HG12	1.84	0.76
1:A:58:ILE:HD11	1:A:71:LEU:HD21	1.71	0.72
1:A:2:VAL:HG22	1:A:316:LEU:HB3	1.74	0.69
1:B:36:VAL:HG13	1:B:77:ALA:HB2	1.77	0.65
1:B:65:ALA:O	1:B:68:GLU:HG3	1.98	0.63
1:A:95:HIS:HD2	1:A:97:VAL:H	1.48	0.61
1:A:158:ARG:HG3	1:A:205:LEU:HD23	1.81	0.61
1:B:235:LEU:HD22	1:B:283:PRO:HB2	1.84	0.60
1:A:273:LEU:HD23	2:A:528(A):HOH:O	2.03	0.59
1:A:2:VAL:HG12	1:A:2:VAL:O	2.01	0.59
1:A:2:VAL:HG11	1:A:313:SER:HA	1.85	0.58
1:A:68:GLU:CG	2:A:592(A):HOH:O	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HB2	1:A:301:TYR:OH	2.04	0.57
1:B:249:ARG:O	1:B:252:LYS:HE3	2.05	0.57
1:A:330:GLU:OE1	1:A:394:ARG:NH1	2.38	0.56
1:B:174:ASN:OD1	2:B:480(B):HOH:O	2.18	0.56
1:A:158:ARG:HD2	2:A:471(A):HOH:O	2.04	0.55
1:A:95:HIS:CD2	1:A:97:VAL:H	2.25	0.54
1:B:62:ALA:HA	1:B:66:GLU:OE1	2.09	0.52
1:A:2:VAL:O	1:A:2:VAL:CG1	2.58	0.50
1:B:319:LYS:O	1:B:323:LEU:HG	2.11	0.50
1:A:355:ALA:O	1:A:359:ASN:HB2	2.12	0.50
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.93	0.50
1:A:23:ASP:HB2	1:A:24:PRO:HD2	1.93	0.50
1:A:16:THR:OG1	1:A:17:VAL:N	2.45	0.48
1:A:68:GLU:HG3	1:A:69:LYS:N	2.27	0.47
1:B:33:LEU:HB2	1:B:301:TYR:HH	1.74	0.47
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.49	0.47
1:B:34:ASP:OD1	1:B:36:VAL:N	2.45	0.46
1:A:37:GLU:OE1	2:A:583(A):HOH:O	2.21	0.46
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.81	0.46
1:A:49:GLY:HA2	1:A:83:LEU:HD22	1.98	0.45
1:A:235:LEU:HG	1:A:240:LEU:CD2	2.47	0.45
1:A:361:SER:HA	2:A:552(A):HOH:O	2.16	0.45
1:B:377:PHE:O	1:B:378:ALA:HB3	2.17	0.45
1:A:261:HIS:NE2	1:B:384:GLN:NE2	2.65	0.44
1:A:336:LYS:HB2	2:A:641(A):HOH:O	2.16	0.44
1:B:185:GLU:HA	1:B:186:PRO:HA	1.77	0.44
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.99	0.43
1:A:192:LEU:N	1:A:193:PRO:HD3	2.34	0.43
1:A:55:ASN:HA	1:A:58:ILE:O	2.19	0.43
1:B:23:ASP:HB2	1:B:24:PRO:HD2	2.01	0.42
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.84	0.42
1:B:294:LYS:HE2	2:B:692(A):HOH:O	2.18	0.42
1:B:2:VAL:HG22	1:B:316:LEU:HB2	2.01	0.42
1:A:394:ARG:HD3	2:A:640(A):HOH:O	2.19	0.42
1:A:181:PRO:HA	2:A:484(A):HOH:O	2.20	0.41
1:A:32:ASN:ND2	2:A:580(A):HOH:O	2.53	0.41
1:A:333:GLU:CD	2:A:642(A):HOH:O	2.50	0.41
1:A:120:HIS:O	1:A:123:ASP:HB2	2.20	0.41
1:B:158:ARG:HG3	1:B:205:LEU:HD23	2.02	0.40
1:A:39:VAL:HG13	1:A:83:LEU:HD12	2.02	0.40
1:B:63:THR:N	1:B:66:GLU:OE1	2.42	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:THR:HG21	1:A:86:PRO:HG2	2.02	0.40
1:A:289:ARG:HD3	2:A:403(A):HOH:O	2.20	0.40

All (3) 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:5:THR:CG2	1:B:374:GLU:OE2[6_655]	1.99	0.21
1:B:343:LEU:CD2	2:B:445(B):HOH:O[4_555]	1.99	0.21
1:B:174:ASN:ND2	2:B:723(B):HOH:O[4_555]	2.16	0.04

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	57
1	B	391/394 (99%)	375 (96%)	13 (3%)	3 (1%)	24	27
All	All	782/788 (99%)	749 (96%)	29 (4%)	4 (0%)	34	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU
1	B	6	PRO
1	B	185	GLU
1	B	23	ASP

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%)	292 (96%)	13 (4%)	35	47
1	B	305/310 (98%)	297 (97%)	8 (3%)	54	71
All	All	610/620 (98%)	589 (97%)	21 (3%)	44	59

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	5	THR
1	A	68	GLU
1	A	94	SER
1	A	127	GLU
1	A	181	PRO
1	A	184	ASN
1	A	213	LEU
1	A	284	LYS
1	A	289	ARG
1	A	330	GLU
1	A	359	ASN
1	A	361	SER
1	B	6	PRO
1	B	68	GLU
1	B	90	THR
1	B	149	ASP
1	B	158	ARG
1	B	235	LEU
1	B	293	TYR
1	B	361	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	184	ASN
1	A	221	GLN
1	A	359	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	384	GLN
1	B	75	ASN
1	B	95	HIS
1	B	221	GLN
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](#)

There are no ligands in this entry.

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.