



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:30 PM GMT

PDB ID : 1XLK
Title : MECHANISM FOR ALDOSE-KETOSE INTERCONVERSION BY D-XYLOSE ISOMERASE INVOLVING RING OPENING FOLLOWED BY A 1,2-HYDRIDE SHIFT
Authors : Collyer, C.A.; Henrick, K.; Blow, D.M.
Deposited on : 1991-10-09
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

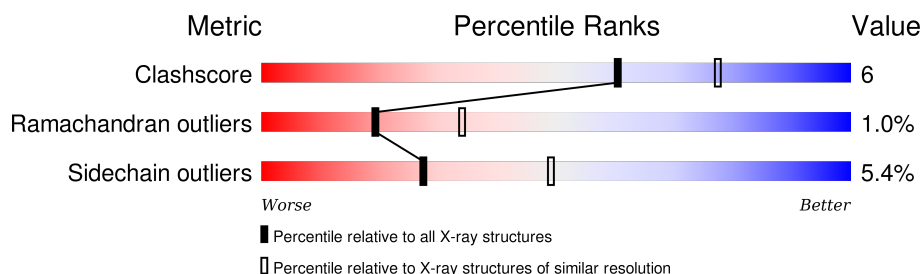
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	394	 68% 28% . .
1	B	394	 65% 27% 6% .

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.

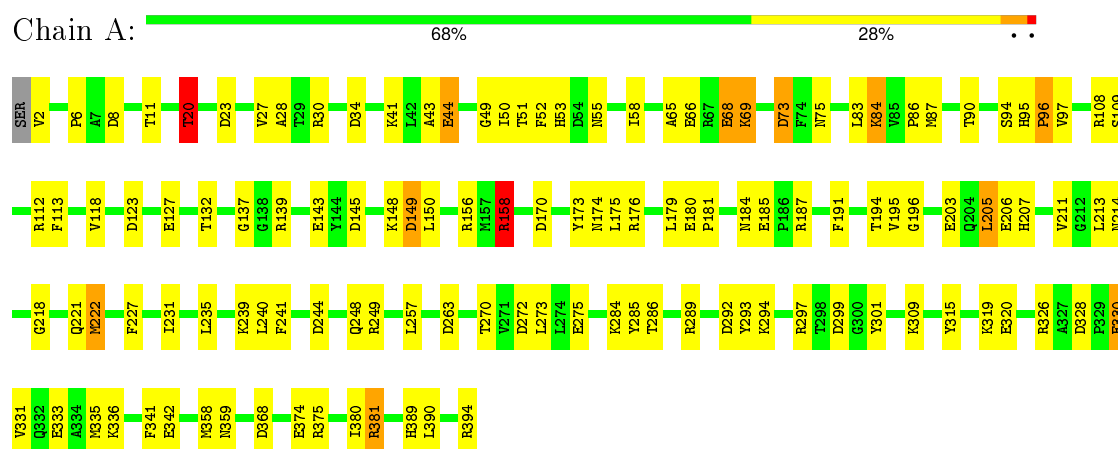
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	256	Total	O	0	0
			256	256		
3	B	266	Total	O	0	0
			266	266		

3 Residue-property plots

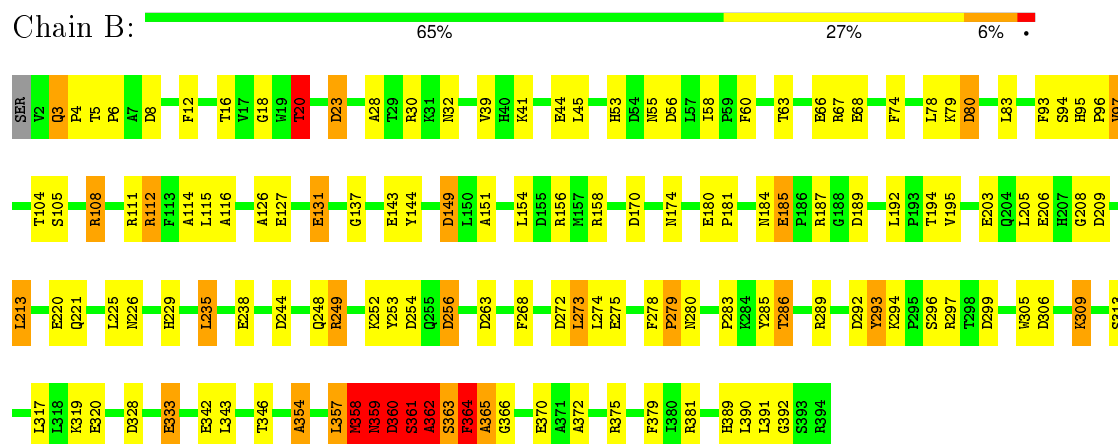
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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	105.80 Å 105.80 Å 154.30 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}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6580	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: 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	1.17	1/3101 (0.0%)	2.36	129/4204 (3.1%)
1	B	1.24	4/3101 (0.1%)	2.32	141/4204 (3.4%)
All	All	1.20	5/6202 (0.1%)	2.34	270/8408 (3.2%)

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	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	361	SER	CA-CB	-13.53	1.32	1.52
1	B	362	ALA	N-CA	-6.21	1.33	1.46
1	A	158	ARG	CD-NE	-5.42	1.37	1.46
1	B	361	SER	C-N	-5.04	1.22	1.34
1	B	370	GLU	CD-OE1	5.02	1.31	1.25

All (270) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	CD-NE-CZ	37.73	176.43	123.60
1	A	108	ARG	NE-CZ-NH1	28.36	134.48	120.30
1	B	361	SER	N-CA-CB	27.07	151.10	110.50
1	A	112	ARG	NE-CZ-NH1	23.07	131.83	120.30
1	A	108	ARG	NE-CZ-NH2	-19.95	110.32	120.30
1	B	358	MET	C-N-CA	19.56	170.61	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ARG	CD-NE-CZ	19.21	150.50	123.60
1	A	112	ARG	NE-CZ-NH2	-17.62	111.49	120.30
1	A	158	ARG	CD-NE-CZ	17.31	147.84	123.60
1	B	361	SER	C-N-CA	15.90	161.45	121.70
1	B	360	ASP	CA-C-N	15.89	152.17	117.20
1	B	108	ARG	NE-CZ-NH1	15.06	127.83	120.30
1	A	139	ARG	NE-CZ-NH1	14.68	127.64	120.30
1	B	30	ARG	NE-CZ-NH2	-14.45	113.08	120.30
1	A	381	ARG	NE-CZ-NH2	-13.79	113.41	120.30
1	A	381	ARG	NE-CZ-NH1	13.73	127.16	120.30
1	B	297	ARG	NE-CZ-NH2	13.36	126.98	120.30
1	A	23	ASP	CB-CG-OD1	13.22	130.20	118.30
1	A	249	ARG	NE-CZ-NH1	12.95	126.77	120.30
1	B	359	ASN	C-N-CA	12.76	153.61	121.70
1	A	187	ARG	NE-CZ-NH1	12.47	126.53	120.30
1	B	30	ARG	NE-CZ-NH1	12.40	126.50	120.30
1	B	358	MET	N-CA-CB	11.98	132.17	110.60
1	B	357	LEU	O-C-N	-11.86	103.72	122.70
1	B	44	GLU	CA-CB-CG	11.65	139.03	113.40
1	A	292	ASP	CB-CG-OD2	11.53	128.68	118.30
1	B	360	ASP	CB-CG-OD2	11.51	128.66	118.30
1	B	379	PHE	CB-CG-CD1	11.44	128.81	120.80
1	A	108	ARG	CD-NE-CZ	11.37	139.51	123.60
1	A	297	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	B	357	LEU	CA-C-N	11.10	141.62	117.20
1	B	292	ASP	CB-CG-OD2	10.97	128.18	118.30
1	A	241	PHE	CB-CG-CD1	10.96	128.48	120.80
1	A	289	ARG	CD-NE-CZ	10.92	138.89	123.60
1	B	170	ASP	CB-CG-OD2	10.91	128.12	118.30
1	A	149	ASP	CB-CG-OD1	10.80	128.02	118.30
1	B	361	SER	CB-CA-C	-10.73	89.70	110.10
1	B	299	ASP	CB-CG-OD1	10.68	127.91	118.30
1	A	289	ARG	NE-CZ-NH2	-10.60	115.00	120.30
1	B	187	ARG	NE-CZ-NH1	10.51	125.56	120.30
1	B	187	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	A	368	ASP	CB-CG-OD2	10.28	127.55	118.30
1	B	357	LEU	C-N-CA	10.18	147.16	121.70
1	B	379	PHE	CB-CG-CD2	-10.16	113.69	120.80
1	B	375	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	B	20	THR	CA-CB-CG2	10.00	126.40	112.40
1	B	108	ARG	CD-NE-CZ	9.99	137.59	123.60
1	B	359	ASN	CB-CA-C	9.90	130.20	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	TYR	CB-CG-CD2	-9.82	115.11	121.00
1	B	289	ARG	NE-CZ-NH2	9.66	125.13	120.30
1	B	108	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	B	273	LEU	CA-CB-CG	9.62	137.43	115.30
1	A	34	ASP	CB-CG-OD1	9.57	126.91	118.30
1	A	187	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	A	394	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	B	360	ASP	O-C-N	-9.48	107.53	122.70
1	B	360	ASP	CA-C-O	-9.43	100.29	120.10
1	B	111	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	A	374	GLU	OE1-CD-OE2	9.23	134.38	123.30
1	B	333	GLU	OE1-CD-OE2	9.18	134.32	123.30
1	B	127	GLU	CA-CB-CG	9.16	133.55	113.40
1	A	123	ASP	CB-CG-OD1	8.96	126.36	118.30
1	A	6	PRO	C-N-CA	8.96	144.09	121.70
1	B	328	ASP	CB-CG-OD1	8.94	126.35	118.30
1	A	145	ASP	CB-CG-OD1	8.89	126.30	118.30
1	B	362	ALA	CA-C-N	8.84	136.65	117.20
1	B	213	LEU	CA-CB-CG	8.78	135.49	115.30
1	B	149	ASP	CB-CG-OD1	8.75	126.18	118.30
1	B	381	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	B	358	MET	CA-CB-CG	-8.67	98.56	113.30
1	A	170	ASP	CB-CG-OD2	-8.61	110.55	118.30
1	A	176	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	A	156	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	A	342	GLU	OE1-CD-OE2	8.24	133.19	123.30
1	A	249	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	B	20	THR	N-CA-CB	-8.24	94.65	110.30
1	B	12	PHE	CB-CG-CD1	-8.20	115.06	120.80
1	A	51	THR	CA-CB-CG2	8.17	123.84	112.40
1	B	23	ASP	CB-CA-C	8.11	126.61	110.40
1	A	68	GLU	OE1-CD-OE2	8.05	132.96	123.30
1	A	342	GLU	CA-CB-CG	7.96	130.92	113.40
1	A	285	TYR	CB-CG-CD1	7.96	125.77	121.00
1	B	391	LEU	C-N-CA	7.95	139.00	122.30
1	B	272	ASP	CB-CG-OD2	7.92	125.43	118.30
1	B	144	TYR	CB-CG-CD2	7.92	125.75	121.00
1	A	299	ASP	CB-CG-OD1	7.84	125.35	118.30
1	B	381	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	285	TYR	CB-CG-CD2	-7.79	116.33	121.00
1	B	189	ASP	CB-CG-OD1	-7.55	111.50	118.30
1	A	8	ASP	CB-CG-OD2	7.43	124.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	TYR	CB-CG-CD1	7.39	125.44	121.00
1	B	362	ALA	N-CA-C	-7.34	91.19	111.00
1	B	244	ASP	CB-CG-OD1	7.33	124.90	118.30
1	B	60	PHE	C-N-CA	7.31	139.98	121.70
1	A	123	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	A	203	GLU	OE1-CD-OE2	-7.27	114.57	123.30
1	B	209	ASP	CB-CG-OD2	7.26	124.83	118.30
1	A	326	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	342	GLU	CB-CA-C	-7.19	96.03	110.40
1	B	144	TYR	CB-CG-CD1	-7.18	116.69	121.00
1	A	375	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	A	176	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	A	156	ARG	CA-CB-CG	7.00	128.79	113.40
1	A	176	ARG	NH1-CZ-NH2	-6.98	111.72	119.40
1	A	320	GLU	CA-CB-CG	6.97	128.73	113.40
1	B	361	SER	CA-CB-OG	6.94	129.94	111.20
1	B	358	MET	CA-C-O	6.93	134.66	120.10
1	B	256	ASP	CB-CG-OD1	6.89	124.50	118.30
1	B	67	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	227	PHE	CB-CG-CD1	-6.85	116.00	120.80
1	A	65	ALA	CB-CA-C	6.83	120.35	110.10
1	B	20	THR	CB-CA-C	6.79	129.92	111.60
1	B	112	ARG	CD-NE-CZ	6.77	133.08	123.60
1	B	342	GLU	OE1-CD-OE2	6.74	131.39	123.30
1	B	208	GLY	O-C-N	-6.74	111.92	122.70
1	B	97	VAL	CA-CB-CG1	6.73	120.99	110.90
1	B	203	GLU	CG-CD-OE2	6.69	131.68	118.30
1	B	80	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	113	PHE	CB-CG-CD2	-6.64	116.15	120.80
1	B	56	ASP	N-CA-CB	6.64	122.54	110.60
1	B	370	GLU	OE1-CD-OE2	6.63	131.26	123.30
1	A	239	LYS	CA-CB-CG	6.63	127.98	113.40
1	B	80	ASP	CB-CG-OD2	-6.62	112.35	118.30
1	A	6	PRO	O-C-N	-6.60	112.14	122.70
1	A	23	ASP	CB-CA-C	6.58	123.56	110.40
1	B	253	TYR	CB-CG-CD2	6.55	124.93	121.00
1	B	8	ASP	CB-CG-OD1	-6.55	112.40	118.30
1	A	139	ARG	NH1-CZ-NH2	-6.53	112.22	119.40
1	A	222	MET	C-N-CA	6.50	137.96	121.70
1	B	306	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	194	THR	CA-CB-CG2	6.47	121.46	112.40
1	A	96	PRO	O-C-N	-6.46	112.36	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	PHE	CB-CG-CD2	-6.41	116.31	120.80
1	A	375	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	A	272	ASP	CB-CG-OD2	6.36	124.02	118.30
1	B	286	THR	N-CA-CB	-6.36	98.22	110.30
1	A	368	ASP	OD1-CG-OD2	-6.34	111.25	123.30
1	B	342	GLU	CG-CD-OE2	-6.33	105.64	118.30
1	B	364	PHE	O-C-N	-6.33	112.57	122.70
1	A	52	PHE	CB-CG-CD2	-6.29	116.40	120.80
1	B	372	ALA	CB-CA-C	6.28	119.51	110.10
1	A	145	ASP	CA-C-O	-6.26	106.95	120.10
1	B	358	MET	CG-SD-CE	6.25	110.20	100.20
1	B	68	GLU	CB-CA-C	6.25	122.90	110.40
1	B	111	ARG	NH1-CZ-NH2	-6.23	112.55	119.40
1	A	145	ASP	CA-C-N	6.21	128.61	116.20
1	A	149	ASP	N-CA-CB	6.20	121.75	110.60
1	A	289	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	297	ARG	N-CA-CB	6.18	121.72	110.60
1	B	362	ALA	CA-C-O	-6.16	107.17	120.10
1	A	263	ASP	CB-CG-OD1	6.15	123.84	118.30
1	A	375	ARG	NH1-CZ-NH2	6.15	126.16	119.40
1	A	273	LEU	CA-CB-CG	6.11	129.36	115.30
1	B	67	ARG	CG-CD-NE	6.10	124.61	111.80
1	B	32	ASN	CA-CB-CG	-6.04	100.11	113.40
1	B	154	LEU	CA-CB-CG	6.03	129.16	115.30
1	B	93	PHE	CA-C-O	-6.01	107.48	120.10
1	A	320	GLU	CG-CD-OE2	6.01	130.31	118.30
1	A	149	ASP	N-CA-C	-6.00	94.80	111.00
1	B	354	ALA	N-CA-CB	6.00	118.49	110.10
1	B	203	GLU	C-N-CA	5.99	136.68	121.70
1	A	301	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	B	192	LEU	CA-CB-CG	5.95	129.00	115.30
1	A	293	TYR	CD1-CE1-CZ	-5.95	114.45	119.80
1	A	30	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	363	SER	O-C-N	-5.86	113.33	122.70
1	A	394	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	170	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	328	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	341	PHE	CB-CG-CD1	-5.79	116.75	120.80
1	B	149	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	B	274	LEU	O-C-N	5.77	131.93	122.70
1	B	363	SER	N-CA-CB	-5.75	101.88	110.50
1	A	20	THR	N-CA-CB	-5.74	99.40	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	CA-C-O	5.72	132.12	120.10
1	B	151	ALA	CB-CA-C	5.70	118.65	110.10
1	A	244	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	118	VAL	CA-CB-CG1	5.70	119.44	110.90
1	B	263	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	362	ALA	O-C-N	-5.69	113.59	122.70
1	B	53	HIS	N-CA-CB	5.67	120.80	110.60
1	B	137	GLY	C-N-CA	5.66	134.19	122.30
1	A	145	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	A	330	GLU	CB-CA-C	-5.65	99.09	110.40
1	A	292	ASP	OD1-CG-OD2	-5.64	112.58	123.30
1	B	149	ASP	N-CA-C	-5.64	95.76	111.00
1	A	30	ARG	CD-NE-CZ	5.63	131.48	123.60
1	A	309	LYS	CA-CB-CG	5.62	125.78	113.40
1	A	297	ARG	CD-NE-CZ	5.62	131.46	123.60
1	B	372	ALA	O-C-N	-5.61	113.72	122.70
1	A	249	ARG	CD-NE-CZ	5.60	131.44	123.60
1	B	206	GLU	CA-CB-CG	5.56	125.63	113.40
1	B	357	LEU	N-CA-C	-5.55	96.00	111.00
1	B	143	GLU	O-C-N	-5.54	113.83	122.70
1	B	289	ARG	CB-CG-CD	5.53	125.99	111.60
1	A	175	LEU	O-C-N	5.52	131.54	122.70
1	B	273	LEU	CB-CG-CD1	5.51	120.36	111.00
1	B	346	THR	CA-CB-OG1	-5.51	97.43	109.00
1	A	173	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	B	320	GLU	OE1-CD-OE2	5.50	129.90	123.30
1	A	211	VAL	CA-CB-CG2	5.48	119.12	110.90
1	B	389	HIS	CA-CB-CG	-5.46	104.31	113.60
1	A	84	LYS	N-CA-CB	-5.45	100.78	110.60
1	A	333	GLU	CA-CB-CG	5.44	125.37	113.40
1	B	249	ARG	CA-C-N	5.44	127.09	116.20
1	A	143	GLU	OE1-CD-OE2	-5.44	116.77	123.30
1	A	96	PRO	CA-C-N	5.43	129.15	117.20
1	B	18	GLY	CA-C-N	5.43	129.15	117.20
1	B	392	GLY	C-N-CA	5.43	135.28	121.70
1	B	363	SER	N-CA-C	5.42	125.64	111.00
1	B	127	GLU	CG-CD-OE2	5.42	129.13	118.30
1	B	174	ASN	CB-CA-C	5.40	121.20	110.40
1	A	270	THR	CA-CB-CG2	5.39	119.95	112.40
1	B	305	TRP	CB-CA-C	5.39	121.18	110.40
1	B	16	THR	OG1-CB-CG2	5.38	122.38	110.00
1	B	285	TYR	CD1-CE1-CZ	-5.37	114.97	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	GLU	OE1-CD-OE2	5.35	129.72	123.30
1	B	189	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	225	LEU	CA-CB-CG	5.34	127.59	115.30
1	B	292	ASP	OD1-CG-OD2	-5.34	113.15	123.30
1	A	389	HIS	CA-CB-CG	-5.34	104.53	113.60
1	A	73	ASP	CA-CB-CG	5.33	125.13	113.40
1	A	2	VAL	CA-CB-CG2	5.33	118.89	110.90
1	A	66	GLU	O-C-N	-5.30	114.22	122.70
1	A	137	GLY	C-N-CA	5.29	133.42	122.30
1	A	205	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	257	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	66	GLU	CG-CD-OE2	5.26	128.82	118.30
1	A	44	GLU	N-CA-CB	5.25	120.05	110.60
1	B	294	LYS	CB-CA-C	-5.24	99.92	110.40
1	A	194	THR	CA-CB-CG2	5.24	119.74	112.40
1	A	293	TYR	CZ-CE2-CD2	-5.24	115.08	119.80
1	B	156	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	127	GLU	OE1-CD-OE2	-5.22	117.03	123.30
1	A	53	HIS	CB-CA-C	-5.22	99.96	110.40
1	A	196	GLY	O-C-N	-5.19	114.40	122.70
1	A	127	GLU	N-CA-CB	5.18	119.92	110.60
1	A	109	SER	CB-CA-C	5.14	119.88	110.10
1	B	143	GLU	CA-C-O	5.14	130.90	120.10
1	A	390	LEU	C-N-CA	5.14	134.55	121.70
1	B	365	ALA	CA-C-N	5.14	126.48	116.20
1	A	342	GLU	N-CA-CB	5.14	119.85	110.60
1	B	293	TYR	CD1-CG-CD2	5.14	123.55	117.90
1	A	27	VAL	CA-CB-CG2	5.13	118.60	110.90
1	A	358	MET	C-N-CA	5.12	134.50	121.70
1	B	280	ASN	CA-C-N	5.12	126.44	116.20
1	A	156	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	208	GLY	C-N-CA	5.11	134.49	121.70
1	A	53	HIS	N-CA-CB	5.10	119.78	110.60
1	B	309	LYS	CA-CB-CG	5.09	124.59	113.40
1	A	286	THR	CA-C-N	5.08	126.37	116.20
1	B	96	PRO	C-N-CA	5.08	134.41	121.70
1	B	297	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	195	VAL	CA-CB-CG1	5.08	118.52	110.90
1	B	391	LEU	CA-CB-CG	5.08	126.98	115.30
1	A	44	GLU	CA-CB-CG	5.06	124.54	113.40
1	B	254	ASP	N-CA-CB	-5.06	101.49	110.60
1	B	293	TYR	CG-CD2-CE2	-5.06	117.25	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	HIS	O-C-N	-5.06	114.60	123.20
1	B	346	THR	CA-CB-CG2	5.05	119.47	112.40
1	B	360	ASP	C-N-CA	-5.04	109.11	121.70
1	A	231	ILE	CA-C-N	5.03	128.27	117.20
1	A	20	THR	CB-CA-C	5.02	125.16	111.60
1	B	361	SER	O-C-N	-5.02	114.66	122.70
1	B	114	ALA	N-CA-CB	-5.02	103.07	110.10
1	B	185	GLU	OE1-CD-OE2	-5.01	117.28	123.30
1	B	126	ALA	CB-CA-C	5.01	117.61	110.10
1	B	279	PRO	O-C-N	-5.01	114.69	122.70
1	A	315	TYR	CB-CG-CD1	5.00	124.00	121.00
1	A	179	LEU	O-C-N	5.00	130.71	122.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	358	MET	Peptide
1	B	359	ASN	Mainchain
1	B	361	SER	Mainchain,Peptide
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	2881	29	0
1	B	3027	0	2876	38	12
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	256	0	0	6	0
3	B	266	0	0	3	5
All	All	6580	0	5757	66	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 6.

All (66) 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:361:SER:HB3	1:B:366:GLY:H	1.40	0.85
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.70	0.72
1:A:95:HIS:HD2	1:A:97:VAL:H	1.37	0.72
1:B:357:LEU:HG	1:B:359:ASN:HA	1.75	0.67
1:B:95:HIS:HD2	1:B:97:VAL:H	1.44	0.64
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.81	0.63
1:B:256:ASP:HB3	1:B:293:TYR:HA	1.81	0.62
1:A:275:GLU:HG3	1:A:319:LYS:HG3	1.82	0.61
1:B:361:SER:CB	1:B:364:PHE:H	2.14	0.60
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.68	0.57
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.86	0.57
1:A:84:LYS:HB2	3:A:660(A):HOH:O	2.03	0.57
1:B:131:GLU:HG3	3:B:649(B):HOH:O	2.04	0.56
1:A:380:ILE:HD11	1:B:296:SER:HB2	1.88	0.55
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.90	0.53
1:A:95:HIS:CD2	1:A:97:VAL:H	2.24	0.53
1:B:361:SER:HB2	1:B:364:PHE:H	1.75	0.52
1:A:20:THR:HG23	1:A:28:ALA:CB	2.40	0.51
1:A:69:LYS:HE2	1:A:73:ASP:OD2	2.12	0.50
1:A:331:VAL:O	1:A:335:MET:HG3	2.11	0.50
1:B:361:SER:HB2	1:B:365:ALA:N	2.27	0.49
1:B:357:LEU:O	1:B:360:ASP:N	2.46	0.49
1:B:360:ASP:OD1	1:B:362:ALA:HB3	2.12	0.49
1:B:195:VAL:HG23	1:B:220:GLU:CD	2.34	0.48
1:B:45:LEU:HB3	1:B:309:LYS:HE3	1.96	0.48
1:B:361:SER:CB	1:B:366:GLY:H	2.18	0.47
1:A:336:LYS:HD3	3:A:635(A):HOH:O	2.14	0.47
1:B:45:LEU:HD22	1:B:309:LYS:HG2	1.96	0.47
1:B:20:THR:HG23	1:B:28:ALA:CB	2.45	0.47
1:B:235:LEU:HD22	1:B:283:PRO:HB2	1.97	0.46
1:B:55:ASN:HA	1:B:58:ILE:O	2.15	0.46
1:A:330:GLU:OE2	1:A:381:ARG:NH2	2.48	0.46
1:A:84:LYS:HD2	3:A:423(A):HOH:O	2.16	0.46
1:B:238:GLU:HG3	3:B:647(B):HOH:O	2.17	0.45
1:B:313:SER:O	1:B:317:LEU:HG	2.16	0.45
1:B:108:ARG:O	1:B:112:ARG:HG3	2.17	0.45
1:B:63:THR:HG23	1:B:66:GLU:OE2	2.17	0.45
1:A:218:GLY:O	1:A:222:MET:HG3	2.18	0.44
1:A:87:MET:HA	1:A:132:THR:O	2.18	0.44
1:A:180:GLU:HA	1:A:181:PRO:HD3	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLU:HA	1:B:181:PRO:HD3	1.78	0.43
1:A:11:THR:HA	1:A:49:GLY:O	2.19	0.43
1:A:20:THR:HG23	1:A:28:ALA:HB2	2.00	0.43
1:B:364:PHE:HB3	3:B:539(B):HOH:O	2.18	0.43
1:A:235:LEU:HG	1:A:240:LEU:HD23	1.99	0.43
1:A:43:ALA:HB2	1:A:83:LEU:HD13	2.01	0.43
1:A:55:ASN:HA	1:A:58:ILE:O	2.19	0.43
1:A:180:GLU:HG3	1:A:214:ASN:O	2.19	0.42
1:B:79:LYS:O	1:B:80:ASP:C	2.55	0.42
1:A:294:LYS:NZ	3:A:466(A):HOH:O	2.52	0.42
1:B:226:ASN:HB3	1:B:229:HIS:HB2	2.01	0.42
1:A:84:LYS:HG3	1:A:86:PRO:HG3	2.02	0.42
1:B:278:PHE:HA	1:B:279:PRO:HD3	1.88	0.42
1:B:158:ARG:HG3	1:B:205:LEU:HD23	2.01	0.42
1:B:354:ALA:O	1:B:358:MET:N	2.53	0.41
1:B:249:ARG:O	1:B:252:LYS:HE3	2.21	0.41
1:A:20:THR:HG23	1:A:28:ALA:HB1	2.01	0.41
1:A:158:ARG:HB3	3:A:459(A):HOH:O	2.20	0.41
1:A:158:ARG:HG2	1:A:205:LEU:HD23	2.03	0.41
1:B:74:PHE:CE2	1:B:78:LEU:HD11	2.56	0.41
1:B:268:PHE:CD1	1:B:390:LEU:HD13	2.55	0.41
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.86	0.40
1:A:75:ASN:ND2	3:A:561(A):HOH:O	2.53	0.40
1:B:221:GLN:HE21	1:B:248:GLN:HB3	1.85	0.40
1:B:360:ASP:O	1:B:363:SER:N	2.51	0.40
1:B:3:GLN:HA	1:B:4:PRO:HD2	1.83	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:116:ALA:CA	1:B:359:ASN:OD1[4_555]	1.25	0.95
1:B:116:ALA:N	1:B:359:ASN:OD1[4_555]	1.30	0.90
1:B:116:ALA:CB	1:B:359:ASN:CB[4_555]	1.39	0.81
1:B:105:SER:CA	3:B:592(B):HOH:O[4_555]	1.53	0.67
1:B:105:SER:N	3:B:592(B):HOH:O[4_555]	1.63	0.57
1:B:116:ALA:CA	1:B:359:ASN:CG[4_555]	1.75	0.45
1:B:104:THR:C	3:B:592(B):HOH:O[4_555]	1.85	0.35
1:B:115:LEU:C	1:B:359:ASN:OD1[4_555]	1.92	0.28
1:B:343:LEU:CD2	3:B:438(B):HOH:O[4_555]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:THR:O	3:B:592(B):HOH:O[4_555]	1.97	0.23
1:B:116:ALA:CA	1:B:359:ASN:CB[4_555]	2.05	0.15
1:B:116:ALA:CB	1:B:359:ASN:CG[4_555]	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%)	376 (96%)	14 (4%)	1 (0%)	46	68
1	B	391/394 (99%)	366 (94%)	18 (5%)	7 (2%)	11	18
All	All	782/788 (99%)	742 (95%)	32 (4%)	8 (1%)	19	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	358	MET
1	B	359	ASN
1	B	360	ASP
1	B	362	ALA
1	A	185	GLU
1	B	185	GLU
1	B	23	ASP
1	B	3	GLN

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%)	288 (94%)	17 (6%)	26	47
1	B	305/310 (98%)	289 (95%)	16 (5%)	29	51
All	All	610/620 (98%)	577 (95%)	33 (5%)	27	49

All (33) 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	50	ILE
1	A	68	GLU
1	A	69	LYS
1	A	90	THR
1	A	94	SER
1	A	96	PRO
1	A	149	ASP
1	A	150	LEU
1	A	158	ARG
1	A	174	ASN
1	A	184	ASN
1	A	213	LEU
1	A	284	LYS
1	A	359	ASN
1	B	5	THR
1	B	6	PRO
1	B	20	THR
1	B	41	LYS
1	B	94	SER
1	B	131	GLU
1	B	149	ASP
1	B	184	ASN
1	B	213	LEU
1	B	235	LEU
1	B	273	LEU
1	B	286	THR
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 (14) 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	359	ASN
1	A	384	GLN
1	B	40	HIS
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 [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 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 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.