



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:30 PM GMT

PDB ID : 1XLI
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

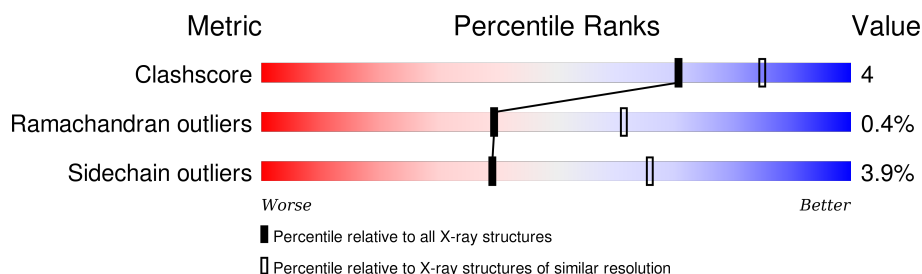
1 Overall quality at a glance

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	 72% 24% . .
1	B	394	 68% 27% . .

2 Entry composition [i](#)

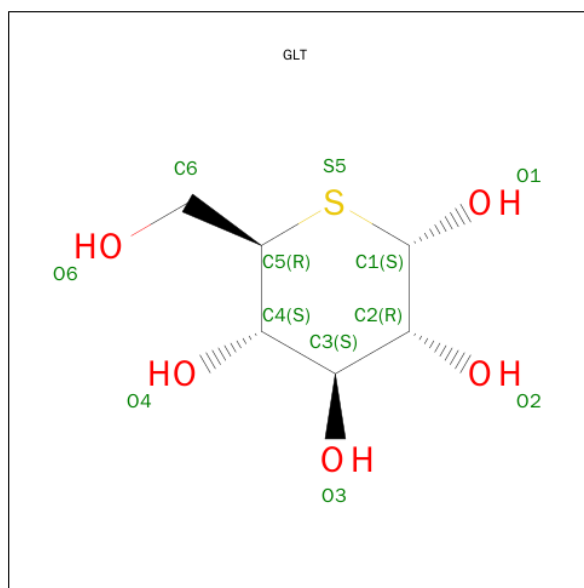
There are 4 unique types of molecules in this entry. The entry contains 6601 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SUGAR (5-DEOXY-5-THIO-ALPHA-D-GLUCOSE) (three-letter code: GLT) (formula: $C_6H_{12}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			12	6	5	1		
2	B	1	Total	C	O	S	0	0
			12	6	5	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is water.

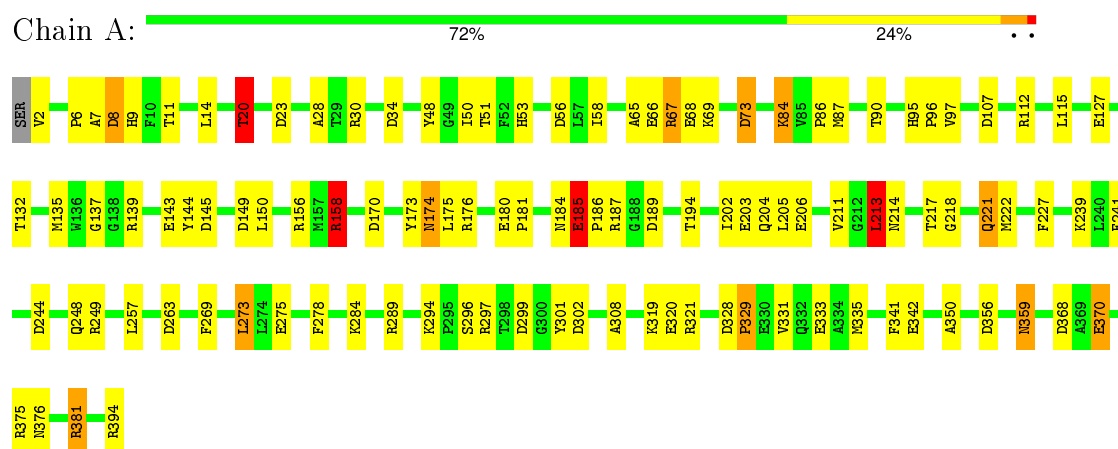
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	255	Total 255	O 255	0	0
4	B	264	Total 264	O 264	0	0

3 Residue-property plots

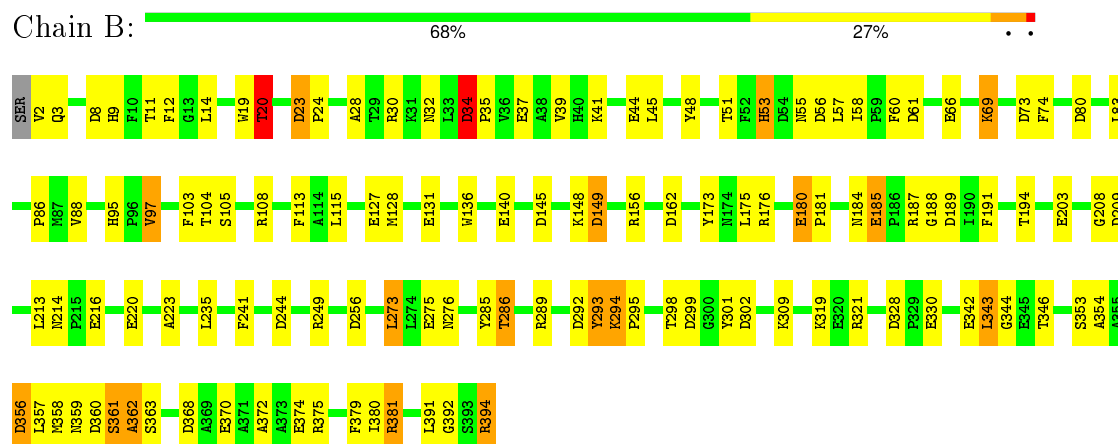
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 153.20 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}	0.150 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6601	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.09	1/3101 (0.0%)	2.15	108/4204 (2.6%)
1	B	1.15	3/3101 (0.1%)	2.06	113/4204 (2.7%)
All	All	1.12	4/6202 (0.1%)	2.11	221/8408 (2.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	361	SER	C-N	17.91	1.75	1.34
1	B	374	GLU	CD-OE1	-5.12	1.20	1.25
1	B	344	GLY	N-CA	-5.04	1.38	1.46
1	A	187	ARG	NE-CZ	5.03	1.39	1.33

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	CD-NE-CZ	25.75	159.66	123.60
1	B	187	ARG	NE-CZ-NH2	-19.49	110.55	120.30
1	A	187	ARG	NE-CZ-NH2	-19.38	110.61	120.30
1	B	361	SER	C-N-CA	18.01	166.74	121.70
1	A	394	ARG	NE-CZ-NH1	16.01	128.31	120.30
1	A	375	ARG	NE-CZ-NH2	-15.78	112.41	120.30
1	B	2	VAL	C-N-CA	14.93	159.01	121.70
1	A	187	ARG	NE-CZ-NH1	13.67	127.14	120.30
1	A	297	ARG	NE-CZ-NH2	-13.61	113.49	120.30
1	A	359	ASN	CA-CB-CG	13.38	142.84	113.40
1	A	23	ASP	CB-CG-OD1	13.16	130.14	118.30
1	A	301	TYR	CB-CG-CD1	-12.67	113.40	121.00
1	A	170	ASP	CB-CG-OD2	-12.58	106.98	118.30
1	A	67	ARG	NE-CZ-NH1	12.57	126.58	120.30
1	B	321	ARG	NE-CZ-NH2	-12.41	114.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ASP	CB-CG-OD2	12.23	129.31	118.30
1	A	249	ARG	NE-CZ-NH1	12.12	126.36	120.30
1	B	356	ASP	O-C-N	-11.99	103.51	122.70
1	A	289	ARG	NE-CZ-NH2	-11.95	114.33	120.30
1	A	112	ARG	CD-NE-CZ	11.94	140.31	123.60
1	A	381	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	A	394	ARG	NE-CZ-NH2	-11.61	114.50	120.30
1	B	375	ARG	NE-CZ-NH2	-11.59	114.50	120.30
1	B	108	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	A	321	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	A	297	ARG	NE-CZ-NH1	10.41	125.51	120.30
1	A	139	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	A	156	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	A	269	PHE	CB-CG-CD1	-9.98	113.82	120.80
1	B	34	ASP	CB-CG-OD1	-9.97	109.32	118.30
1	B	358	MET	C-N-CA	9.95	146.58	121.70
1	B	356	ASP	CA-C-N	9.89	138.96	117.20
1	B	361	SER	O-C-N	-9.82	107.00	122.70
1	B	127	GLU	CA-CB-CG	9.81	134.99	113.40
1	A	241	PHE	CB-CG-CD1	9.71	127.59	120.80
1	A	342	GLU	CA-CB-CG	9.68	134.69	113.40
1	B	299	ASP	CB-CG-OD1	9.39	126.75	118.30
1	B	34	ASP	CB-CG-OD2	9.29	126.66	118.30
1	A	139	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	B	30	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	A	8	ASP	CB-CG-OD2	8.99	126.39	118.30
1	B	360	ASP	CB-CG-OD2	8.99	126.39	118.30
1	A	269	PHE	CB-CG-CD2	8.79	126.95	120.80
1	B	220	GLU	OE1-CD-OE2	8.76	133.81	123.30
1	A	34	ASP	CB-CG-OD2	8.72	126.15	118.30
1	A	170	ASP	CB-CG-OD1	8.54	125.99	118.30
1	B	381	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	B	73	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	B	213	LEU	CA-CB-CG	8.47	134.79	115.30
1	A	273	LEU	CA-CB-CG	8.44	134.71	115.30
1	A	299	ASP	CB-CG-OD1	8.35	125.81	118.30
1	B	273	LEU	CA-CB-CG	8.33	134.46	115.30
1	A	107	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	B	381	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	73	ASP	CB-CG-OD2	-7.97	111.13	118.30
1	A	6	PRO	C-N-CA	7.89	141.43	121.70
1	A	302	ASP	CB-CG-OD2	-7.87	111.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	THR	N-CA-CB	-7.85	95.38	110.30
1	A	68	GLU	OE1-CD-OE2	7.85	132.72	123.30
1	A	342	GLU	N-CA-CB	7.83	124.69	110.60
1	A	176	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	B	162	ASP	CB-CG-OD1	7.80	125.32	118.30
1	B	244	ASP	CB-CG-OD1	7.80	125.32	118.30
1	B	128	MET	CG-SD-CE	7.79	112.67	100.20
1	A	112	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	A	145	ASP	CB-CG-OD1	7.75	125.28	118.30
1	B	368	ASP	CB-CG-OD1	7.71	125.23	118.30
1	B	23	ASP	CB-CA-C	7.68	125.76	110.40
1	A	51	THR	CA-CB-CG2	7.61	123.06	112.40
1	A	56	ASP	CB-CG-OD2	7.54	125.09	118.30
1	B	108	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	B	361	SER	CA-C-N	7.45	133.59	117.20
1	B	97	VAL	CA-CB-CG1	7.35	121.92	110.90
1	B	115	LEU	CB-CA-C	7.28	124.03	110.20
1	B	20	THR	N-CA-CB	-7.26	96.50	110.30
1	A	156	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	B	356	ASP	C-N-CA	7.03	139.26	121.70
1	B	293	TYR	CB-CG-CD2	-6.97	116.82	121.00
1	B	8	ASP	CB-CG-OD2	6.96	124.56	118.30
1	B	249	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	B	241	PHE	CB-CG-CD2	-6.87	115.99	120.80
1	A	143	GLU	OE1-CD-OE2	-6.86	115.06	123.30
1	B	189	ASP	CB-CG-OD2	6.85	124.47	118.30
1	B	156	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	145	ASP	CB-CG-OD1	6.82	124.44	118.30
1	B	162	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	A	8	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	A	368	ASP	CB-CG-OD1	6.70	124.33	118.30
1	B	113	PHE	CB-CG-CD2	-6.67	116.13	120.80
1	A	23	ASP	CB-CA-C	6.66	123.72	110.40
1	B	342	GLU	OE1-CD-OE2	6.65	131.28	123.30
1	A	321	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	149	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	239	LYS	CA-CB-CG	6.58	127.88	113.40
1	B	359	ASN	CA-CB-CG	6.58	127.88	113.40
1	B	185	GLU	OE1-CD-OE2	-6.58	115.41	123.30
1	A	342	GLU	OE1-CD-OE2	6.57	131.19	123.30
1	A	203	GLU	OE1-CD-OE2	-6.57	115.42	123.30
1	A	289	ARG	CD-NE-CZ	6.55	132.77	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	TYR	CB-CG-CD1	6.54	124.92	121.00
1	A	53	HIS	N-CA-CB	6.52	122.33	110.60
1	B	60	PHE	C-N-CA	6.52	138.00	121.70
1	B	294	LYS	CA-CB-CG	6.50	127.70	113.40
1	A	65	ALA	CB-CA-C	6.47	119.80	110.10
1	B	88	VAL	CG1-CB-CG2	-6.44	100.60	110.90
1	A	320	GLU	CG-CD-OE2	6.40	131.10	118.30
1	B	44	GLU	CG-CD-OE1	-6.37	105.56	118.30
1	A	297	ARG	CD-NE-CZ	6.37	132.52	123.60
1	A	370	GLU	CG-CD-OE1	-6.36	105.58	118.30
1	B	328	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	127	GLU	OE1-CD-OE2	-6.30	115.73	123.30
1	B	391	LEU	C-N-CA	6.27	135.48	122.30
1	B	30	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	298	THR	O-C-N	-6.25	112.70	122.70
1	B	372	ALA	O-C-N	-6.25	112.70	122.70
1	B	48	TYR	N-CA-CB	-6.21	99.42	110.60
1	B	187	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	B	363	SER	CB-CA-C	6.17	121.81	110.10
1	B	249	ARG	CD-NE-CZ	6.16	132.23	123.60
1	B	180	GLU	CG-CD-OE1	6.16	130.61	118.30
1	A	67	ARG	CD-NE-CZ	6.12	132.17	123.60
1	B	149	ASP	N-CA-C	-6.09	94.55	111.00
1	B	379	PHE	CB-CG-CD2	-6.06	116.56	120.80
1	B	343	LEU	C-N-CA	6.05	135.00	122.30
1	B	187	ARG	NH1-CZ-NH2	6.04	126.05	119.40
1	B	131	GLU	CG-CD-OE1	6.04	130.38	118.30
1	B	208	GLY	O-C-N	-6.03	113.06	122.70
1	B	342	GLU	CG-CD-OE2	-6.02	106.25	118.30
1	A	301	TYR	CG-CD1-CE1	-5.98	116.52	121.30
1	B	362	ALA	N-CA-C	-5.98	94.85	111.00
1	B	48	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	A	149	ASP	N-CA-CB	5.96	121.32	110.60
1	B	175	LEU	CB-CA-C	-5.94	98.91	110.20
1	A	341	PHE	CA-C-N	5.94	130.27	117.20
1	A	115	LEU	CB-CA-C	5.92	121.45	110.20
1	A	375	ARG	NH1-CZ-NH2	5.82	125.80	119.40
1	B	359	ASN	CB-CA-C	5.80	122.00	110.40
1	A	144	TYR	CB-CG-CD1	-5.79	117.52	121.00
1	B	53	HIS	N-CA-CB	5.73	120.92	110.60
1	A	342	GLU	CB-CA-C	-5.72	98.95	110.40
1	B	51	THR	CA-CB-CG2	5.69	120.37	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	GLU	CA-CB-CG	5.68	125.91	113.40
1	B	32	ASN	CA-CB-CG	-5.68	100.89	113.40
1	A	20	THR	N-CA-CB	-5.67	99.53	110.30
1	B	379	PHE	CB-CG-CD1	5.66	124.76	120.80
1	A	244	ASP	CA-CB-CG	5.65	125.84	113.40
1	B	220	GLU	CG-CD-OE2	-5.64	107.02	118.30
1	B	189	ASP	CB-CG-OD1	-5.64	113.23	118.30
1	B	203	GLU	CG-CD-OE2	5.63	129.56	118.30
1	B	372	ALA	CB-CA-C	5.63	118.55	110.10
1	A	294	LYS	CG-CD-CE	5.63	128.79	111.90
1	B	44	GLU	CG-CD-OE2	5.62	129.55	118.30
1	A	6	PRO	O-C-N	-5.61	113.72	122.70
1	B	34	ASP	CB-CA-C	5.60	121.60	110.40
1	B	256	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	149	ASP	N-CA-C	-5.59	95.89	111.00
1	A	221	GLN	O-C-N	-5.56	113.81	122.70
1	A	127	GLU	CA-CB-CG	5.55	125.61	113.40
1	B	394	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	158	ARG	CD-NE-CZ	5.52	131.33	123.60
1	A	30	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	289	ARG	CD-NE-CZ	5.49	131.29	123.60
1	A	34	ASP	OD1-CG-OD2	-5.48	112.89	123.30
1	A	96	PRO	O-C-N	-5.48	113.93	122.70
1	A	308	ALA	CA-C-O	5.47	131.59	120.10
1	B	188	GLY	O-C-N	-5.46	113.96	122.70
1	B	176	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	221	GLN	C-N-CA	5.44	135.31	121.70
1	B	223	ALA	C-N-CA	5.44	133.72	122.30
1	A	185	GLU	OE1-CD-OE2	-5.42	116.80	123.30
1	A	137	GLY	C-N-CA	5.39	133.63	122.30
1	A	194	THR	CA-CB-CG2	5.38	119.93	112.40
1	A	301	TYR	CA-C-O	-5.36	108.84	120.10
1	A	257	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	214	ASN	CB-CG-ND2	5.34	129.52	116.70
1	A	174	ASN	N-CA-CB	5.34	120.21	110.60
1	A	23	ASP	OD1-CG-OD2	-5.33	113.18	123.30
1	A	320	GLU	CG-CD-OE1	-5.33	107.64	118.30
1	B	302	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	175	LEU	CA-CB-CG	5.31	127.52	115.30
1	B	103	PHE	CB-CG-CD1	5.30	124.51	120.80
1	A	189	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	213	LEU	CA-CB-CG	5.29	127.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	LYS	CA-CB-CG	5.28	125.02	113.40
1	B	301	TYR	CG-CD2-CE2	-5.27	117.08	121.30
1	B	12	PHE	CB-CG-CD1	-5.26	117.11	120.80
1	B	140	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	B	20	THR	CA-CB-CG2	5.25	119.75	112.40
1	B	194	THR	CA-CB-CG2	5.22	119.70	112.40
1	A	211	VAL	CA-CB-CG2	5.21	118.71	110.90
1	B	209	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	297	ARG	O-C-N	-5.20	114.38	122.70
1	B	2	VAL	CA-C-O	5.19	131.00	120.10
1	A	203	GLU	CG-CD-OE2	5.19	128.67	118.30
1	A	329	PRO	C-N-CA	5.18	134.65	121.70
1	B	358	MET	CG-SD-CE	5.18	108.49	100.20
1	B	354	ALA	N-CA-CB	5.18	117.35	110.10
1	B	80	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	B	128	MET	CA-CB-CG	5.17	122.09	113.30
1	A	376	ASN	N-CA-CB	5.16	119.88	110.60
1	A	189	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	B	370	GLU	CG-CD-OE1	-5.14	108.02	118.30
1	A	84	LYS	C-N-CA	5.14	134.54	121.70
1	A	350	ALA	N-CA-CB	-5.13	102.92	110.10
1	B	19	TRP	N-CA-CB	5.12	119.83	110.60
1	B	66	GLU	CG-CD-OE1	-5.11	108.08	118.30
1	A	48	TYR	CB-CG-CD2	5.11	124.07	121.00
1	A	263	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	37	GLU	CB-CG-CD	5.10	127.97	114.20
1	A	356	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	206	GLU	OE1-CD-OE2	5.08	129.40	123.30
1	B	216	GLU	CG-CD-OE2	-5.07	108.17	118.30
1	A	7	ALA	C-N-CA	5.06	134.34	121.70
1	B	173	TYR	CB-CG-CD1	5.05	124.03	121.00
1	A	289	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	B	285	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	A	66	GLU	O-C-N	-5.02	114.66	122.70
1	B	392	GLY	C-N-CA	5.02	134.25	121.70
1	A	241	PHE	CB-CG-CD2	-5.02	117.29	120.80
1	B	346	THR	CA-CB-OG1	-5.01	98.47	109.00
1	B	256	ASP	CB-CG-OD1	5.00	122.80	118.30

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	3027	0	2881	26	1
1	B	3027	0	2879	27	7
2	A	12	0	10	0	0
2	B	12	0	11	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	255	0	0	3	2
4	B	264	0	0	2	7
All	All	6601	0	5781	52	9

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 (52) 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:C	1:B:362:ALA:N	1.75	1.38
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.58	0.82
1:A:58:ILE:HD13	1:A:67:ARG:HD2	1.73	0.71
1:A:95:HIS:HD2	1:A:97:VAL:H	1.41	0.67
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.76	0.67
1:B:95:HIS:HD2	1:B:97:VAL:H	1.41	0.66
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.78	0.66
1:A:158:ARG:HG3	1:A:205:LEU:HD23	1.82	0.62
1:B:45:LEU:HB3	1:B:309:LYS:HE3	1.83	0.59
1:A:84:LYS:HD2	4:A:424(A):HOH:O	2.03	0.58
1:A:69:LYS:HE2	1:A:73:ASP:OD2	2.05	0.57
1:B:20:THR:HG23	1:B:28:ALA:CB	2.36	0.56
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.88	0.56
1:B:23:ASP:HB2	1:B:24:PRO:HD2	1.88	0.55
1:B:55:ASN:HA	1:B:58:ILE:O	2.07	0.55
1:A:275:GLU:HG3	1:A:319:LYS:HG3	1.90	0.52
1:B:45:LEU:HD22	1:B:309:LYS:HE3	1.92	0.52
1:A:84:LYS:HB2	4:A:654(A):HOH:O	2.10	0.51
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:HIS:CD2	1:A:97:VAL:H	2.26	0.50
1:B:148:LYS:HG3	1:B:191:PHE:HZ	1.77	0.49
1:B:57:LEU:HD11	1:B:74:PHE:CD1	2.47	0.49
1:B:381:ARG:HD3	4:B:795(B):HOH:O	2.14	0.47
1:A:87:MET:HA	1:A:132:THR:O	2.15	0.47
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.96	0.47
1:B:20:THR:HG22	4:B:811(B):HOH:O	2.14	0.46
1:A:8:ASP:O	1:A:9:HIS:HB2	2.15	0.46
1:A:14:LEU:HD13	1:A:50:ILE:HD11	1.98	0.46
1:A:296:SER:H	1:B:380:ILE:HD11	1.81	0.45
1:B:330:GLU:OE1	1:B:394:ARG:NH1	2.50	0.44
1:B:34:ASP:HA	1:B:35:PRO:HD3	1.79	0.44
1:B:14:LEU:HD21	1:B:35:PRO:HB3	2.00	0.44
1:B:180:GLU:HA	1:B:181:PRO:HD3	1.77	0.44
1:B:294:LYS:HA	1:B:295:PRO:HD3	1.86	0.43
1:B:23:ASP:CB	1:B:24:PRO:HD2	2.47	0.43
1:A:273:LEU:HD21	1:A:278:PHE:CE1	2.54	0.43
1:B:136:TRP:HB2	2:B:400:GLT:H61	1.99	0.43
1:B:53:HIS:O	1:B:56:ASP:HB2	2.19	0.43
1:A:217:THR:HA	1:A:227:PHE:CD1	2.54	0.43
1:A:218:GLY:O	1:A:222:MET:HG3	2.19	0.43
1:A:158:ARG:HD3	1:A:204:GLN:O	2.19	0.42
1:A:20:THR:HG23	1:A:28:ALA:CB	2.49	0.42
1:A:20:THR:HG23	1:A:28:ALA:HB2	1.99	0.42
1:A:331:VAL:O	1:A:335:MET:HG3	2.19	0.42
1:B:180:GLU:HG3	1:B:214:ASN:O	2.20	0.42
1:A:185:GLU:HA	1:A:186:PRO:HA	1.81	0.42
1:A:202:ILE:HD11	1:A:213:LEU:HD23	2.01	0.42
1:A:328:ASP:HA	1:A:329:PRO:HD3	1.86	0.42
1:A:180:GLU:HA	1:A:181:PRO:HD3	1.79	0.42
1:B:353:SER:H	1:B:356:ASP:HB2	1.83	0.41
1:A:381:ARG:HG3	4:A:593(A):HOH:O	2.21	0.41
1:B:35:PRO:O	1:B:39:VAL:HG23	2.20	0.40

All (9) 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:CA	4:B:846(B):HOH:O[4_555]	1.16	1.04
1:B:105:SER:N	4:B:846(B):HOH:O[4_555]	1.32	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:564(A):HOH:O	4:B:668(B):HOH:O[4_555]	1.81	0.39
4:B:761(B):HOH:O	4:B:829(B):HOH:O[4_555]	1.90	0.30
1:B:104:THR:C	4:B:846(B):HOH:O[4_555]	1.92	0.28
1:A:69:LYS:NZ	1:B:276:ASN:O[6_665]	1.97	0.23
1:B:343:LEU:CD2	4:B:697(B):HOH:O[4_555]	2.05	0.15
1:B:9:HIS:CE1	4:A:648(A):HOH:O[6_655]	2.11	0.09
1:B:104:THR:O	4:B:846(B):HOH:O[4_555]	2.18	0.02

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%)	371 (95%)	19 (5%)	1 (0%)	46	68
1	B	391/394 (99%)	376 (96%)	13 (3%)	2 (0%)	34	55
All	All	782/788 (99%)	747 (96%)	32 (4%)	3 (0%)	39	61

All (3) Ramachandran outliers are listed below:

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

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%)	39	66
1	B	305/310 (98%)	293 (96%)	12 (4%)	39	66
All	All	610/620 (98%)	586 (96%)	24 (4%)	39	66

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	20	THR
1	A	90	THR
1	A	135	MET
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	A	370	GLU
1	B	20	THR
1	B	34	ASP
1	B	41	LYS
1	B	61	ASP
1	B	69	LYS
1	B	149	ASP
1	B	184	ASN
1	B	235	LEU
1	B	273	LEU
1	B	286	THR
1	B	293	TYR
1	B	357	LEU

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	120	HIS
1	A	174	ASN
1	A	184	ASN
1	A	221	GLN

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Mol	Chain	Res	Type
1	A	384	GLN
1	B	40	HIS
1	B	75	ASN
1	B	76	GLN
1	B	95	HIS
1	B	184	ASN
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](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	GLT	A	400	3	10,12,12	1.81	3 (30%)	11,17,17	3.03	5 (45%)
2	GLT	B	400	3	10,12,12	0.93	0	11,17,17	2.76	6 (54%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLT	A	400	3	-	0/1/22/22	0/1/1/1
2	GLT	B	400	3	-	0/1/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	GLT	C4-C5	-3.53	1.50	1.53
2	A	400	GLT	C6-C5	-2.14	1.50	1.52
2	A	400	GLT	C5-S5	2.75	1.86	1.82

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	GLT	O4-C4-C5	-3.41	101.04	108.83
2	A	400	GLT	O1-C1-C2	2.07	114.78	110.11
2	B	400	GLT	O2-C2-C1	2.34	114.99	110.43
2	A	400	GLT	O2-C2-C1	2.61	115.51	110.43
2	B	400	GLT	O1-C1-C2	2.91	116.67	110.11
2	B	400	GLT	C4-C3-C2	3.58	117.47	110.79
2	B	400	GLT	O3-C3-C2	3.83	118.96	110.34
2	A	400	GLT	C4-C3-C2	4.09	118.43	110.79
2	A	400	GLT	C1-C2-C3	4.61	120.91	110.69
2	B	400	GLT	C1-C2-C3	4.96	121.68	110.69
2	A	400	GLT	O3-C3-C2	6.70	125.42	110.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	GLT	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.