Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 07:00 PM EST

PDB ID	:	1XLF
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

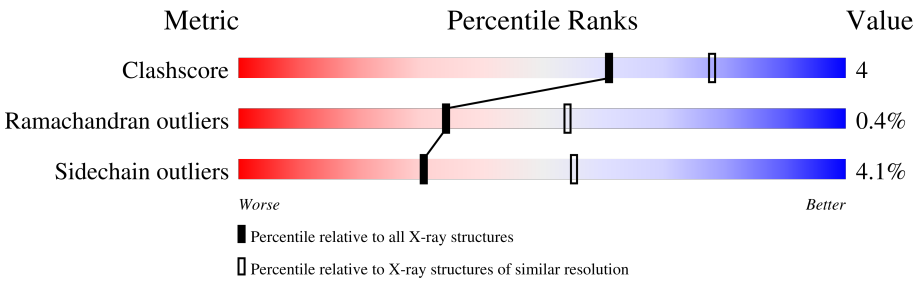
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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 of 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	394	66% 29% .
1	B	394	68% 28% . .

2 Entry composition (i)

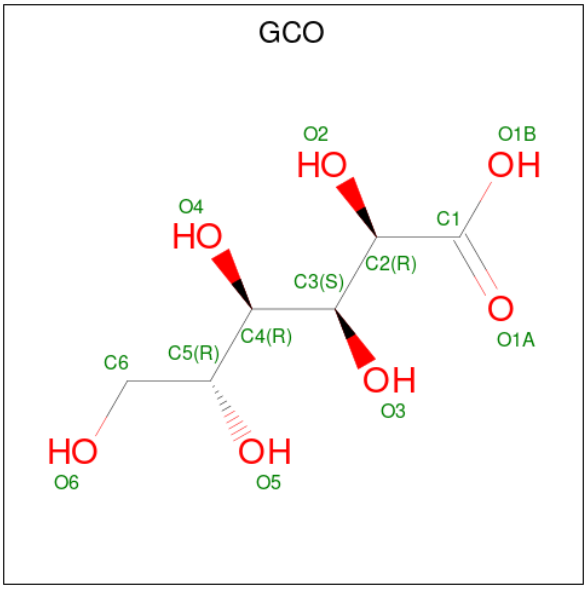
There are 4 unique types of molecules in this entry. The entry contains 6599 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	393	3027	1919	520	579	9	0	0	0
1	B	393	3027	1919	520	579	9	0	0	0

- Molecule 2 is D-gluconic acid (three-letter code: GCO) (formula: $C_6H_{12}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	13	6	7	0	0
2	B	1	13	6	7	0	0

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	253	253	253	0	0
			Total	O		
4	B	262	262	262	0	0

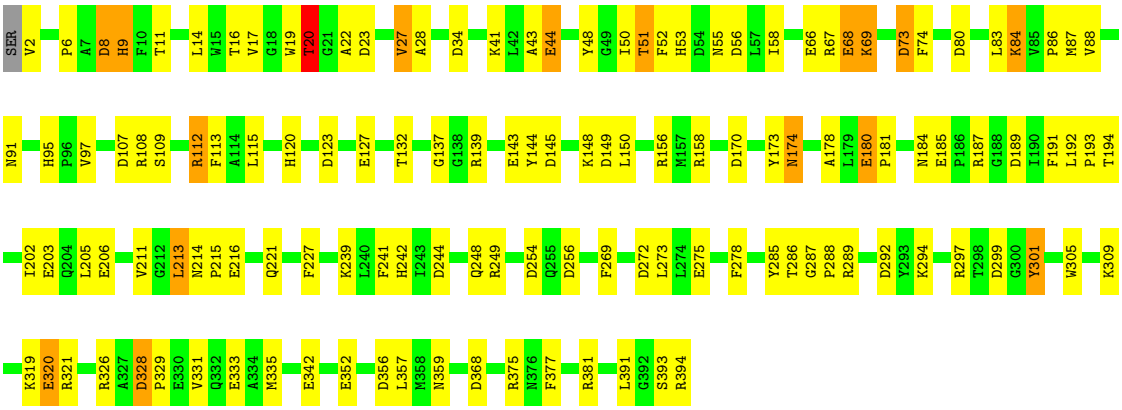
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

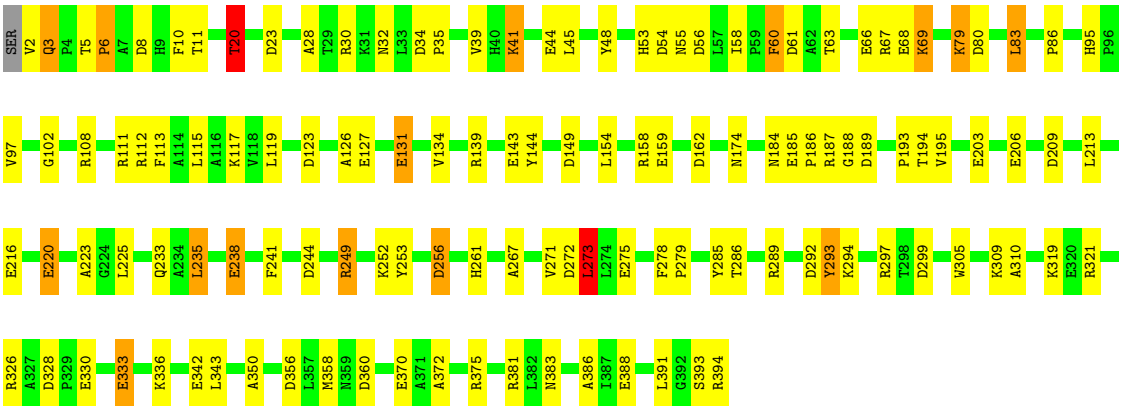
• Molecule 1: D-XYLOSE ISOMERASE

Chain A: 66% 29%



• Molecule 1: D-XYLOSE ISOMERASE

Chain B: 68% 28%



4 Data and refinement statistics (i)

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	106.00Å 106.00Å 153.80Å 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}	0.152 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6599	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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: GCO, 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	1.19	0/3101	2.21	131/4204 (3.1%)
1	B	1.22	2/3101 (0.1%)	2.13	134/4204 (3.2%)
All	All	1.20	2/6202 (0.0%)	2.17	265/8408 (3.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	220	GLU	CD-OE1	-5.56	1.19	1.25
1	B	393	SER	CB-OG	-5.16	1.35	1.42

All (265) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	394	ARG	CD-NE-CZ	33.81	170.94	123.60
1	A	8	ASP	CB-CG-OD2	14.68	131.51	118.30
1	B	381	ARG	NE-CZ-NH2	-13.73	113.44	120.30
1	A	297	ARG	NE-CZ-NH2	-13.33	113.64	120.30
1	B	30	ARG	NE-CZ-NH1	13.04	126.82	120.30
1	A	249	ARG	NE-CZ-NH1	12.93	126.76	120.30
1	B	244	ASP	CB-CG-OD1	12.90	129.91	118.30
1	A	23	ASP	CB-CG-OD1	12.76	129.78	118.30
1	B	187	ARG	NE-CZ-NH2	-12.41	114.09	120.30
1	A	68	GLU	OE1-CD-OE2	12.26	138.01	123.30
1	A	187	ARG	NE-CZ-NH2	-11.98	114.31	120.30
1	B	30	ARG	NE-CZ-NH2	-11.89	114.35	120.30
1	B	293	TYR	CB-CG-CD2	-11.89	113.86	121.00
1	B	187	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	A	187	ARG	NE-CZ-NH1	11.37	125.99	120.30
1	B	108	ARG	NE-CZ-NH2	-11.17	114.72	120.30
1	A	241	PHE	CB-CG-CD1	10.91	128.44	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	381	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	B	60	PHE	C-N-CA	10.79	148.66	121.70
1	A	156	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	A	342	GLU	OE1-CD-OE2	10.71	136.15	123.30
1	B	328	ASP	CB-CG-OD1	10.60	127.84	118.30
1	B	213	LEU	CA-CB-CG	10.54	139.54	115.30
1	A	108	ARG	NE-CZ-NH1	10.13	125.36	120.30
1	B	108	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	A	394	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	B	326	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	A	368	ASP	CB-CG-OD2	9.76	127.08	118.30
1	B	127	GLU	CA-CB-CG	9.73	134.81	113.40
1	B	360	ASP	CB-CG-OD2	9.73	127.06	118.30
1	B	249	ARG	NE-CZ-NH1	9.65	125.13	120.30
1	A	73	ASP	CB-CG-OD2	-9.53	109.72	118.30
1	A	6	PRO	C-N-CA	9.33	145.02	121.70
1	B	143	GLU	OE1-CD-OE2	-9.19	112.27	123.30
1	A	326	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	A	158	ARG	CD-NE-CZ	9.15	136.41	123.60
1	A	299	ASP	CB-CG-OD1	9.10	126.49	118.30
1	A	139	ARG	NE-CZ-NH2	9.06	124.83	120.30
1	B	189	ASP	CB-CG-OD2	9.04	126.44	118.30
1	A	34	ASP	CB-CG-OD1	8.87	126.28	118.30
1	A	113	PHE	CB-CG-CD2	-8.85	114.61	120.80
1	B	333	GLU	OE1-CD-OE2	8.84	133.90	123.30
1	B	108	ARG	CD-NE-CZ	8.82	135.95	123.60
1	A	269	PHE	CB-CG-CD1	-8.74	114.68	120.80
1	B	292	ASP	CB-CG-OD2	8.52	125.97	118.30
1	B	44	GLU	CG-CD-OE1	-8.46	101.38	118.30
1	B	297	ARG	NE-CZ-NH2	8.42	124.51	120.30
1	B	20	THR	N-CA-CB	-8.18	94.75	110.30
1	B	289	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	B	299	ASP	CB-CG-OD1	8.06	125.56	118.30
1	A	375	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	A	112	ARG	CB-CG-CD	7.91	132.18	111.60
1	B	206	GLU	CA-CB-CG	7.89	130.77	113.40
1	A	67	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A	381	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	143	GLU	OE1-CD-OE2	-7.76	113.99	123.30
1	B	321	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	A	285	TYR	CB-CG-CD2	-7.69	116.39	121.00
1	A	368	ASP	OD1-CG-OD2	-7.67	108.72	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	342	GLU	CA-CB-CG	7.67	130.26	113.40
1	A	216	GLU	CG-CD-OE1	7.65	133.61	118.30
1	A	73	ASP	CB-CG-OD1	7.58	125.12	118.30
1	A	215	PRO	O-C-N	7.44	134.61	122.70
1	A	320	GLU	CA-CB-CG	7.43	129.76	113.40
1	B	115	LEU	CB-CA-C	7.42	124.30	110.20
1	A	292	ASP	CB-CG-OD2	7.39	124.96	118.30
1	B	134	VAL	CA-CB-CG1	7.37	121.96	110.90
1	B	23	ASP	CB-CA-C	7.36	125.12	110.40
1	B	370	GLU	OE1-CD-OE2	7.35	132.12	123.30
1	B	162	ASP	CB-CG-OD1	7.34	124.90	118.30
1	A	51	THR	CA-CB-CG2	7.33	122.66	112.40
1	A	6	PRO	O-C-N	-7.30	111.02	122.70
1	B	342	GLU	CG-CD-OE2	-7.30	103.70	118.30
1	A	149	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	2	VAL	C-N-CA	7.25	139.82	121.70
1	A	342	GLU	N-CA-CB	7.14	123.45	110.60
1	B	69	LYS	CA-CB-CG	7.03	128.87	113.40
1	B	203	GLU	CG-CD-OE2	7.01	132.32	118.30
1	A	84	LYS	CA-CB-CG	7.01	128.81	113.40
1	A	256	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	321	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	B	273	LEU	CA-CB-CG	6.99	131.38	115.30
1	A	27	VAL	CA-CB-CG2	6.93	121.30	110.90
1	A	301	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	A	112	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	A	269	PHE	CB-CG-CD2	6.89	125.62	120.80
1	B	249	ARG	CA-C-N	6.88	129.97	116.20
1	B	326	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	170	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	A	333	GLU	CA-CB-CG	6.79	128.34	113.40
1	A	249	ARG	CD-NE-CZ	6.78	133.10	123.60
1	A	211	VAL	CA-CB-CG2	6.78	121.06	110.90
1	A	23	ASP	CB-CA-C	6.78	123.95	110.40
1	B	67	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	A	173	TYR	CB-CG-CD1	6.76	125.06	121.00
1	B	23	ASP	CB-CG-OD2	6.76	124.38	118.30
1	A	174	ASN	CA-CB-CG	6.75	128.25	113.40
1	A	48	TYR	CB-CG-CD1	-6.73	116.97	121.00
1	B	159	GLU	CA-CB-CG	6.72	128.18	113.40
1	B	220	GLU	OE1-CD-OE2	6.72	131.36	123.30
1	A	149	ASP	N-CA-CB	6.71	122.68	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	216	GLU	CG-CD-OE2	-6.69	104.92	118.30
1	B	144	TYR	CB-CG-CD1	-6.68	116.99	121.00
1	B	34	ASP	CB-CG-OD2	6.67	124.31	118.30
1	B	149	ASP	CB-CG-OD1	6.67	124.31	118.30
1	B	44	GLU	CG-CD-OE2	6.64	131.58	118.30
1	A	145	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	20	THR	N-CA-CB	-6.61	97.74	110.30
1	B	375	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	B	67	ARG	CG-CD-NE	6.54	125.54	111.80
1	B	69	LYS	CD-CE-NZ	6.54	126.75	111.70
1	B	238	GLU	CA-CB-CG	6.54	127.78	113.40
1	B	391	LEU	C-N-CA	6.53	136.01	122.30
1	A	368	ASP	CB-CG-OD1	6.48	124.13	118.30
1	B	68	GLU	CB-CA-C	6.47	123.35	110.40
1	A	144	TYR	CB-CG-CD1	-6.45	117.13	121.00
1	B	113	PHE	CB-CG-CD1	6.44	125.31	120.80
1	A	357	LEU	CB-CG-CD2	-6.39	100.13	111.00
1	A	173	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	A	294	LYS	CD-CE-NZ	-6.37	97.04	111.70
1	A	342	GLU	CB-CA-C	-6.36	97.67	110.40
1	B	238	GLU	CB-CG-CD	6.34	131.32	114.20
1	A	174	ASN	OD1-CG-ND2	6.34	136.48	121.90
1	B	162	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	A	80	ASP	CB-CG-OD1	6.31	123.98	118.30
1	B	113	PHE	CB-CG-CD2	-6.30	116.39	120.80
1	B	154	LEU	CB-CA-C	6.29	122.15	110.20
1	A	149	ASP	N-CA-C	-6.29	94.03	111.00
1	A	393	SER	C-N-CA	6.27	137.37	121.70
1	B	249	ARG	O-C-N	-6.26	112.55	123.20
1	B	6	PRO	CA-C-N	6.26	130.97	117.20
1	B	53	HIS	N-CA-CB	6.25	121.86	110.60
1	A	67	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	189	ASP	CB-CG-OD1	-6.19	112.73	118.30
1	B	79	LYS	O-C-N	-6.17	112.83	122.70
1	B	372	ALA	O-C-N	-6.15	112.86	122.70
1	B	186	PRO	N-CA-C	6.15	128.09	112.10
1	A	328	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	342	GLU	OE1-CD-OE2	6.10	130.62	123.30
1	A	289	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	112	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	B	193	PRO	O-C-N	-6.09	112.96	122.70
1	B	119	LEU	CB-CA-C	6.07	121.73	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	56	ASP	N-CA-CB	6.06	121.50	110.60
1	A	8	ASP	CB-CG-OD1	-6.05	112.86	118.30
1	B	123	ASP	CB-CG-OD2	6.04	123.73	118.30
1	B	272	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	272	ASP	O-C-N	-6.00	113.09	122.70
1	A	66	GLU	O-C-N	-5.99	113.12	122.70
1	A	194	THR	CA-CB-CG2	5.98	120.78	112.40
1	B	388	GLU	O-C-N	-5.98	113.13	122.70
1	B	372	ALA	CB-CA-C	5.97	119.06	110.10
1	A	254	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	A	241	PHE	CB-CG-CD2	-5.95	116.64	120.80
1	A	19	TRP	CA-C-O	5.92	132.53	120.10
1	A	297	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	194	THR	CA-CB-CG2	5.90	120.66	112.40
1	A	115	LEU	CB-CA-C	5.89	121.40	110.20
1	B	32	ASN	CA-CB-CG	-5.86	100.51	113.40
1	B	174	ASN	C-N-CA	5.85	136.33	121.70
1	A	53	HIS	N-CA-CB	5.84	121.12	110.60
1	A	342	GLU	CG-CD-OE2	-5.84	106.62	118.30
1	A	203	GLU	CG-CD-OE2	5.83	129.97	118.30
1	B	188	GLY	C-N-CA	5.80	136.19	121.70
1	B	279	PRO	O-C-N	-5.79	113.43	122.70
1	B	386	ALA	N-CA-CB	5.79	118.20	110.10
1	A	22	ALA	CB-CA-C	5.79	118.78	110.10
1	A	189	ASP	CB-CG-OD2	5.77	123.49	118.30
1	B	83	LEU	CA-CB-CG	5.77	128.57	115.30
1	B	356	ASP	CB-CG-OD2	5.76	123.49	118.30
1	B	330	GLU	CG-CD-OE2	5.74	129.78	118.30
1	B	10	PHE	CB-CG-CD1	5.73	124.81	120.80
1	A	91	ASN	CB-CG-OD1	5.73	133.06	121.60
1	A	206	GLU	N-CA-CB	5.73	120.91	110.60
1	A	74	PHE	CB-CG-CD2	-5.72	116.80	120.80
1	A	297	ARG	O-C-N	-5.71	113.57	122.70
1	A	109	SER	CB-CA-C	5.70	120.93	110.10
1	B	8	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	A	127	GLU	CA-CB-CG	5.68	125.89	113.40
1	B	394	ARG	CG-CD-NE	-5.67	99.88	111.80
1	A	113	PHE	CB-CG-CD1	5.66	124.76	120.80
1	B	20	THR	CA-CB-CG2	5.64	120.30	112.40
1	B	216	GLU	CG-CD-OE1	5.64	129.58	118.30
1	B	209	ASP	CB-CG-OD1	-5.63	113.23	118.30
1	A	286	THR	CA-C-N	5.62	127.44	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	358	MET	C-N-CA	5.60	135.70	121.70
1	A	52	PHE	CB-CG-CD1	5.58	124.71	120.80
1	A	66	GLU	CG-CD-OE2	5.57	129.45	118.30
1	A	273	LEU	CA-CB-CG	5.57	128.12	115.30
1	B	350	ALA	N-CA-CB	5.57	117.89	110.10
1	B	328	ASP	OD1-CG-OD2	-5.56	112.73	123.30
1	A	391	LEU	C-N-CA	5.55	133.95	122.30
1	A	112	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	B	206	GLU	CG-CD-OE2	-5.50	107.30	118.30
1	B	126	ALA	CB-CA-C	5.50	118.34	110.10
1	B	48	TYR	N-CA-CB	-5.48	100.73	110.60
1	B	278	PHE	N-CA-CB	-5.48	100.73	110.60
1	B	383	ASN	O-C-N	-5.48	113.94	122.70
1	B	158	ARG	NE-CZ-NH1	-5.47	117.57	120.30
1	B	154	LEU	CA-CB-CG	5.45	127.84	115.30
1	B	294	LYS	CD-CE-NZ	-5.43	99.20	111.70
1	B	256	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	B	293	TYR	CB-CG-CD1	5.43	124.26	121.00
1	B	391	LEU	O-C-N	-5.42	113.98	123.20
1	B	5	THR	CA-CB-CG2	5.42	119.99	112.40
1	A	107	ASP	CA-C-O	5.42	131.48	120.10
1	B	3	GLN	N-CA-CB	5.41	120.34	110.60
1	B	203	GLU	O-C-N	-5.40	114.06	122.70
1	A	377	PHE	CA-C-N	5.40	129.08	117.20
1	A	112	ARG	CG-CD-NE	5.39	123.13	111.80
1	A	278	PHE	CB-CG-CD1	-5.39	117.03	120.80
1	B	203	GLU	OE1-CD-OE2	-5.38	116.84	123.30
1	A	137	GLY	C-N-CA	5.38	133.60	122.30
1	A	356	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	239	LYS	CA-CB-CG	5.37	125.22	113.40
1	B	20	THR	CB-CA-C	5.36	126.08	111.60
1	B	285	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	B	253	TYR	CB-CG-CD2	5.35	124.21	121.00
1	B	310	ALA	O-C-N	-5.35	114.14	122.70
1	A	244	ASP	CA-CB-CG	5.34	125.16	113.40
1	B	375	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	88	VAL	CA-CB-CG2	5.33	118.89	110.90
1	A	107	ASP	CA-CB-CG	5.33	125.11	113.40
1	B	381	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	14	LEU	O-C-N	-5.31	114.20	122.70
1	A	180	GLU	CG-CD-OE1	5.31	128.92	118.30
1	B	393	SER	CB-CA-C	5.30	120.16	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	297	ARG	C-N-CA	5.29	134.92	121.70
1	A	391	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	139	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	261	HIS	C-N-CA	5.25	133.32	122.30
1	A	56	ASP	N-CA-CB	5.23	120.01	110.60
1	A	203	GLU	OE1-CD-OE2	-5.23	117.02	123.30
1	B	60	PHE	O-C-N	-5.22	114.35	122.70
1	A	127	GLU	N-CA-CB	5.22	119.99	110.60
1	B	292	ASP	OD1-CG-OD2	-5.21	113.39	123.30
1	A	67	ARG	CG-CD-NE	-5.20	100.87	111.80
1	B	111	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	297	ARG	CD-NE-CZ	5.20	130.88	123.60
1	A	52	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	B	241	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	B	189	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	B	297	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	B	203	GLU	C-N-CA	5.16	134.60	121.70
1	A	213	LEU	CD1-CG-CD2	-5.15	95.04	110.50
1	A	352	GLU	N-CA-C	-5.14	97.11	111.00
1	B	54	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	44	GLU	CA-C-N	5.13	128.50	117.20
1	A	227	PHE	CB-CG-CD1	-5.13	117.21	120.80
1	B	330	GLU	CG-CD-OE1	-5.12	108.07	118.30
1	A	305	TRP	CB-CA-C	5.11	120.61	110.40
1	A	178	ALA	CB-CA-C	5.07	117.71	110.10
1	B	249	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	23	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	320	GLU	CG-CD-OE2	5.07	128.43	118.30
1	A	127	GLU	CB-CA-C	-5.06	100.28	110.40
1	A	272	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	102	GLY	N-CA-C	-5.05	100.47	113.10
1	B	370	GLU	CG-CD-OE1	-5.05	108.20	118.30
1	B	127	GLU	CG-CD-OE2	5.04	128.38	118.30
1	B	225	LEU	CB-CG-CD1	5.04	119.56	111.00
1	A	216	GLU	OE1-CD-OE2	-5.04	117.26	123.30
1	B	233	GLN	CB-CG-CD	5.03	124.67	111.60
1	A	287	GLY	CA-C-O	5.02	129.63	120.60
1	B	223	ALA	O-C-N	-5.01	114.69	123.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	31	0
1	B	3027	0	2880	22	1
2	A	13	0	10	0	0
2	B	13	0	11	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	253	0	0	6	0
4	B	262	0	0	3	1
All	All	6599	0	5782	53	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 (53) 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:275:GLU:HG3	1:B:319:LYS:HG3	1.63	0.80
1:A:95:HIS:HD2	1:A:97:VAL:H	1.37	0.71
1:A:84:LYS:HB2	4:A:675(A):HOH:O	1.94	0.68
1:B:95:HIS:HD2	1:B:97:VAL:H	1.41	0.67
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.79	0.65
1:A:84:LYS:HD2	4:A:548(A):HOH:O	2.03	0.59
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.85	0.58
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.68	0.57
1:A:20:THR:HG23	1:A:28:ALA:HB1	1.87	0.56
1:A:84:LYS:HG3	1:A:86:PRO:HG3	1.86	0.56
1:B:20:THR:HG23	1:B:28:ALA:CB	2.35	0.56
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.87	0.54
1:A:27:VAL:HG21	4:A:960(B):HOH:O	2.07	0.54
1:B:238:GLU:HG3	4:B:1012(B):HOH:O	2.08	0.54
1:A:95:HIS:CD2	1:A:97:VAL:H	2.23	0.53
1:A:20:THR:HG23	1:A:28:ALA:CB	2.39	0.52
1:A:275:GLU:HG3	1:A:319:LYS:HG3	1.90	0.52
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.75	0.52
1:A:8:ASP:O	1:A:9:HIS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LEU:HD22	1:B:309:LYS:HE3	1.93	0.50
1:B:55:ASN:HA	1:B:58:ILE:O	2.13	0.49
1:B:249:ARG:O	1:B:252:LYS:HE3	2.15	0.47
1:A:328:ASP:HA	1:A:329:PRO:HD3	1.80	0.47
1:A:43:ALA:HB2	1:A:83:LEU:HD13	1.98	0.46
1:B:45:LEU:HB3	1:B:309:LYS:HE3	1.96	0.46
1:A:120:HIS:O	1:A:123:ASP:HB2	2.15	0.46
1:B:35:PRO:O	1:B:39:VAL:HG23	2.16	0.46
1:A:331:VAL:O	1:A:335:MET:HG3	2.16	0.46
1:A:69:LYS:HE2	1:A:73:ASP:OD2	2.16	0.46
1:B:63:THR:HG23	1:B:66:GLU:OE2	2.17	0.45
1:B:131:GLU:HG3	4:B:1014(B):HOH:O	2.16	0.45
1:A:55:ASN:HA	1:A:58:ILE:O	2.17	0.45
1:B:60:PHE:HE1	1:B:117:LYS:HE3	1.82	0.45
1:A:180:GLU:HG3	1:A:214:ASN:O	2.18	0.44
1:A:20:THR:HB	4:A:695(A):HOH:O	2.17	0.44
1:A:180:GLU:HA	1:A:181:PRO:HD3	1.74	0.44
1:A:181:PRO:HA	4:A:1006(A):HOH:O	2.17	0.44
1:B:195:VAL:HG23	1:B:220:GLU:CD	2.37	0.44
1:A:11:THR:HG21	1:A:86:PRO:HG2	2.01	0.43
1:A:309:LYS:HB2	1:A:309:LYS:HE2	1.67	0.43
1:B:69:LYS:HE2	4:B:919(B):HOH:O	2.17	0.43
1:B:41:LYS:HG2	1:B:305:TRP:CE2	2.54	0.42
1:A:87:MET:HA	1:A:132:THR:O	2.19	0.42
1:A:242:HIS:CD2	1:A:288:PRO:HG2	2.54	0.42
1:A:50:ILE:HG12	1:A:51:THR:N	2.35	0.42
1:B:267:ALA:O	1:B:271:VAL:HG23	2.20	0.42
1:B:256:ASP:HB3	1:B:293:TYR:HA	2.02	0.42
1:A:192:LEU:N	1:A:193:PRO:HD3	2.35	0.41
1:A:202:ILE:O	1:A:205:LEU:HB2	2.21	0.41
1:A:301:TYR:HD2	4:A:534(A):HOH:O	2.03	0.41
1:B:79:LYS:O	1:B:80:ASP:C	2.59	0.41
1:A:16:THR:OG1	1:A:17:VAL:N	2.54	0.41
1:B:235:LEU:HD12	1:B:273:LEU:HD11	2.03	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)
1:B:343:LEU:CD2	4:B:1017(B):HOH:O[4_555]	2.06	0.14

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	391/394 (99%)	374 (96%)	16 (4%)	1 (0%)	41	61
1	B	391/394 (99%)	371 (95%)	18 (5%)	2 (0%)	29	48
All	All	782/788 (99%)	745 (95%)	34 (4%)	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	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%)	291 (95%)	14 (5%)	27	50
1	B	305/310 (98%)	294 (96%)	11 (4%)	35	61
All	All	610/620 (98%)	585 (96%)	25 (4%)	30	55

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	9	HIS
1	A	20	THR

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Mol	Chain	Res	Type
1	A	41	LYS
1	A	44	GLU
1	A	68	GLU
1	A	69	LYS
1	A	112	ARG
1	A	150	LEU
1	A	174	ASN
1	A	184	ASN
1	A	213	LEU
1	A	320	GLU
1	A	359	ASN
1	B	6	PRO
1	B	20	THR
1	B	41	LYS
1	B	61	ASP
1	B	131	GLU
1	B	184	ASN
1	B	235	LEU
1	B	273	LEU
1	B	286	THR
1	B	333	GLU
1	B	336	LYS

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

Mol	Chain	Res	Type
1	A	75	ASN
1	A	95	HIS
1	A	120	HIS
1	A	184	ASN
1	A	221	GLN
1	A	359	ASN
1	A	384	GLN
1	B	40	HIS
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 monosaccharides 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	GCO	A	400	3	12,12,12	0.74	0	16,16,16	1.25	1 (6%)
2	GCO	B	400	3	12,12,12	1.52	2 (16%)	16,16,16	3.27	9 (56%)

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	GCO	A	400	3	-	7/18/18/18	-
2	GCO	B	400	3	-	5/18/18/18	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	GCO	C5-C4	-3.04	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	GCO	O4-C4	2.12	1.48	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	400	GCO	O5-C5-C6	-7.15	92.36	109.14
2	B	400	GCO	O3-C3-C4	5.16	121.48	109.47
2	B	400	GCO	O1B-C1-C2	3.94	123.92	113.27
2	B	400	GCO	C3-C2-C1	3.80	114.09	109.32
2	B	400	GCO	C4-C3-C2	-3.54	107.33	113.60
2	A	400	GCO	C3-C2-C1	3.51	113.73	109.32
2	B	400	GCO	O6-C6-C5	-3.24	104.02	111.07
2	B	400	GCO	C6-C5-C4	3.12	119.17	112.41
2	B	400	GCO	O1A-C1-C2	-2.78	114.31	121.63
2	B	400	GCO	O5-C5-C4	2.58	115.38	109.10

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	GCO	C3-C4-C5-C6
2	A	400	GCO	C3-C4-C5-O5
2	A	400	GCO	O4-C4-C5-O5
2	B	400	GCO	C3-C4-C5-C6
2	A	400	GCO	O4-C4-C5-C6
2	B	400	GCO	C2-C3-C4-C5
2	B	400	GCO	C2-C3-C4-O4
2	B	400	GCO	O3-C3-C4-O4
2	B	400	GCO	O3-C3-C4-C5
2	A	400	GCO	O3-C3-C4-C5
2	A	400	GCO	O3-C3-C4-O4
2	A	400	GCO	C2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.