



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:30 PM GMT

PDB ID : 1XLD
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

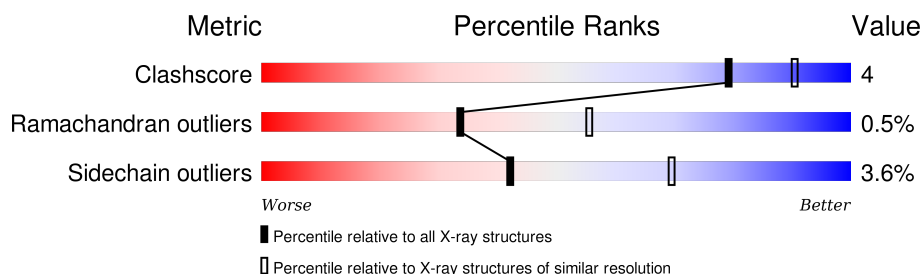
1 Overall quality at a glance

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	
1	B	394	

2 Entry composition [i](#)

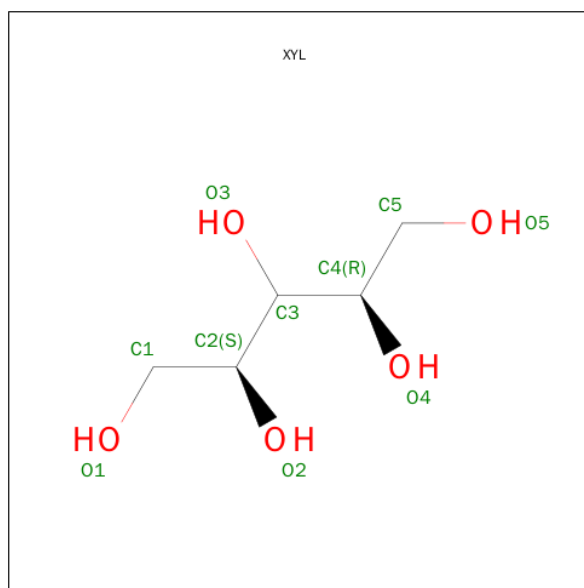
There are 4 unique types of molecules in this entry. The entry contains 6578 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (D-XYLOSE (LINEAR FORM)) (three-letter code: XYL) (formula: $C_5H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		

- 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.

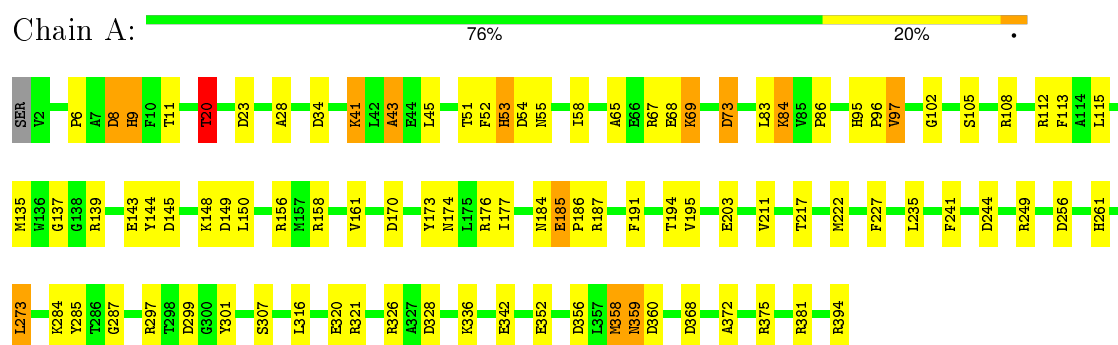
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	247	Total 247	O 247	0	0
4	B	253	Total 253	O 253	0	0

3 Residue-property plots

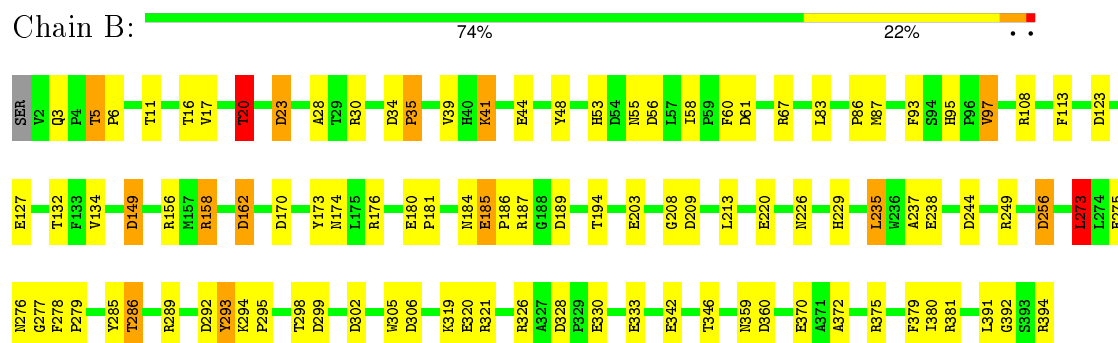
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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	105.60 Å 105.60 Å 153.50 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.148 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6578	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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, XYL

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	1.07	0/3101	2.14	92/4204 (2.2%)
1	B	1.09	2/3101 (0.1%)	1.98	93/4204 (2.2%)
All	All	1.08	2/6202 (0.0%)	2.06	185/8408 (2.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	GLU	CB-CG	6.51	1.64	1.52
1	B	277	GLY	N-CA	5.89	1.54	1.46

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	CD-NE-CZ	27.05	161.46	123.60
1	A	394	ARG	NE-CZ-NH1	23.68	132.14	120.30
1	B	381	ARG	NE-CZ-NH2	-21.73	109.43	120.30
1	B	187	ARG	NE-CZ-NH2	-17.40	111.60	120.30
1	A	67	ARG	CD-NE-CZ	16.40	146.57	123.60
1	A	187	ARG	NE-CZ-NH2	-16.33	112.13	120.30
1	A	375	ARG	NE-CZ-NH2	-15.41	112.60	120.30
1	A	187	ARG	NE-CZ-NH1	15.15	127.88	120.30
1	A	249	ARG	NE-CZ-NH1	13.98	127.29	120.30
1	A	394	ARG	NE-CZ-NH2	-13.49	113.55	120.30
1	A	108	ARG	NE-CZ-NH1	13.46	127.03	120.30
1	B	187	ARG	NE-CZ-NH1	13.12	126.86	120.30
1	A	297	ARG	NE-CZ-NH2	-12.85	113.88	120.30
1	A	67	ARG	NE-CZ-NH1	12.79	126.69	120.30
1	A	359	ASN	CA-CB-CG	12.60	141.11	113.40
1	B	256	ASP	CB-CG-OD1	12.42	129.48	118.30
1	B	381	ARG	NE-CZ-NH1	12.29	126.44	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	B	326	ARG	NE-CZ-NH2	-11.35	114.63	120.30
1	A	342	GLU	CA-CB-CG	11.18	137.99	113.40
1	B	375	ARG	NE-CZ-NH2	-10.87	114.87	120.30
1	A	149	ASP	CB-CG-OD1	10.46	127.71	118.30
1	B	108	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	A	34	ASP	CB-CG-OD1	10.17	127.45	118.30
1	B	321	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	B	209	ASP	CB-CG-OD2	10.09	127.38	118.30
1	A	8	ASP	CB-CG-OD2	9.85	127.16	118.30
1	B	123	ASP	CB-CG-OD2	9.79	127.11	118.30
1	A	112	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	A	256	ASP	CB-CG-OD1	9.44	126.80	118.30
1	A	241	PHE	CB-CG-CD1	9.21	127.25	120.80
1	A	23	ASP	CB-CG-OD1	9.11	126.50	118.30
1	A	144	TYR	CB-CG-CD1	-8.98	115.61	121.00
1	B	244	ASP	CB-CG-OD1	8.92	126.33	118.30
1	A	173	TYR	CB-CG-CD1	8.88	126.33	121.00
1	A	73	ASP	CB-CG-OD2	-8.71	110.46	118.30
1	A	6	PRO	C-N-CA	8.67	143.38	121.70
1	B	30	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	A	301	TYR	CB-CG-CD2	-8.57	115.86	121.00
1	A	342	GLU	N-CA-CB	8.50	125.91	110.60
1	B	127	GLU	CA-CB-CG	8.45	131.99	113.40
1	B	20	THR	N-CA-CB	-8.33	94.48	110.30
1	A	51	THR	CA-CB-CG2	8.30	124.02	112.40
1	A	145	ASP	CB-CG-OD1	8.27	125.75	118.30
1	B	213	LEU	CA-CB-CG	8.25	134.28	115.30
1	A	67	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	A	149	ASP	N-CA-CB	8.06	125.11	110.60
1	B	34	ASP	CB-CG-OD2	8.03	125.53	118.30
1	A	176	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	A	299	ASP	CB-CG-OD1	7.85	125.37	118.30
1	B	379	PHE	CB-CG-CD1	7.83	126.28	120.80
1	B	256	ASP	CB-CG-OD2	-7.82	111.26	118.30
1	A	68	GLU	OE1-CD-OE2	7.77	132.63	123.30
1	A	241	PHE	CB-CG-CD2	-7.69	115.42	120.80
1	B	44	GLU	CG-CD-OE1	-7.59	103.12	118.30
1	B	289	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	A	144	TYR	CB-CG-CD2	7.47	125.48	121.00
1	B	156	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	372	ALA	O-C-N	-7.44	110.80	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	B	328	ASP	CB-CG-OD1	7.41	124.97	118.30
1	B	394	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	A	273	LEU	CA-CB-CG	7.36	132.22	115.30
1	B	299	ASP	CB-CG-OD1	7.32	124.88	118.30
1	B	293	TYR	CB-CG-CD2	-7.26	116.64	121.00
1	B	60	PHE	C-N-CA	7.21	139.73	121.70
1	B	113	PHE	CB-CG-CD2	-7.12	115.81	120.80
1	A	261	HIS	C-N-CA	7.12	137.25	122.30
1	A	321	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	B	23	ASP	CB-CA-C	6.93	124.26	110.40
1	B	189	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	A	8	ASP	CB-CG-OD1	-6.85	112.13	118.30
1	A	139	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	372	ALA	CB-CA-C	6.82	120.33	110.10
1	A	6	PRO	O-C-N	-6.74	111.92	122.70
1	A	113	PHE	CB-CG-CD2	-6.65	116.14	120.80
1	B	286	THR	N-CA-CB	-6.65	97.67	110.30
1	A	342	GLU	OE1-CD-OE2	6.61	131.23	123.30
1	B	372	ALA	O-C-N	-6.60	112.14	122.70
1	A	23	ASP	CB-CA-C	6.57	123.54	110.40
1	A	115	LEU	CB-CA-C	6.56	122.66	110.20
1	B	185	GLU	OE1-CD-OE2	-6.53	115.47	123.30
1	A	211	VAL	CA-CB-CG2	6.52	120.68	110.90
1	B	108	ARG	CD-NE-CZ	6.52	132.73	123.60
1	A	108	ARG	CD-NE-CZ	6.51	132.72	123.60
1	B	249	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	176	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	170	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	B	162	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	B	306	ASP	CB-CG-OD2	6.41	124.07	118.30
1	B	330	GLU	CG-CD-OE1	-6.35	105.60	118.30
1	A	149	ASP	N-CA-C	-6.31	93.96	111.00
1	B	330	GLU	CG-CD-OE2	6.31	130.91	118.30
1	B	5	THR	CA-CB-CG2	6.30	121.22	112.40
1	B	97	VAL	CA-CB-CG1	6.26	120.29	110.90
1	B	346	THR	CA-CB-OG1	-6.20	95.97	109.00
1	B	360	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	56	ASP	N-CA-CB	6.20	121.76	110.60
1	B	170	ASP	CB-CG-OD2	6.19	123.87	118.30
1	B	302	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	B	238	GLU	CA-CB-CG	-6.15	99.87	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	379	PHE	CB-CG-CD2	-6.14	116.50	120.80
1	A	20	THR	N-CA-CB	-6.11	98.70	110.30
1	A	173	TYR	CB-CG-CD2	-6.09	117.34	121.00
1	B	162	ASP	CB-CG-OD1	6.08	123.78	118.30
1	A	381	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	342	GLU	CB-CA-C	-6.06	98.28	110.40
1	B	149	ASP	CB-CG-OD1	6.05	123.75	118.30
1	B	333	GLU	CA-CB-CG	6.04	126.69	113.40
1	B	292	ASP	CB-CG-OD2	6.03	123.73	118.30
1	B	108	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	B	203	GLU	CG-CD-OE2	5.99	130.27	118.30
1	B	370	GLU	OE1-CD-OE2	5.97	130.46	123.30
1	B	194	THR	CA-CB-CG2	5.91	120.67	112.40
1	B	158	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	B	209	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	B	44	GLU	CG-CD-OE2	5.88	130.06	118.30
1	A	320	GLU	CG-CD-OE2	5.86	130.02	118.30
1	B	149	ASP	N-CA-C	-5.84	95.23	111.00
1	A	137	GLY	C-N-CA	5.84	134.56	122.30
1	A	244	ASP	CA-CB-CG	5.83	126.24	113.40
1	B	392	GLY	C-N-CA	5.83	136.28	121.70
1	B	298	THR	C-N-CA	5.83	136.27	121.70
1	A	156	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	174	ASN	C-N-CA	5.81	136.22	121.70
1	A	53	HIS	N-CA-CB	5.80	121.04	110.60
1	B	185	GLU	CG-CD-OE2	5.80	129.90	118.30
1	A	375	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	273	LEU	CA-CB-CG	5.78	128.59	115.30
1	B	289	ARG	CD-NE-CZ	5.77	131.68	123.60
1	A	297	ARG	CD-NE-CZ	5.77	131.67	123.60
1	A	96	PRO	CA-C-N	5.75	129.85	117.20
1	A	356	ASP	CB-CG-OD2	5.74	123.47	118.30
1	B	326	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	B	359	ASN	CB-CA-C	5.64	121.68	110.40
1	A	84	LYS	CA-CB-CG	5.64	125.80	113.40
1	B	134	VAL	CA-CB-CG1	5.55	119.23	110.90
1	A	43	ALA	CB-CA-C	5.54	118.42	110.10
1	B	237	ALA	C-N-CA	5.52	135.50	121.70
1	A	368	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	328	ASP	OD1-CG-OD2	-5.51	112.82	123.30
1	A	194	THR	CA-CB-CG2	5.50	120.09	112.40
1	B	23	ASP	CB-CG-OD1	5.48	123.23	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	GLU	CA-CB-CG	5.47	125.44	113.40
1	A	297	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	48	TYR	N-CA-CB	-5.45	100.78	110.60
1	B	53	HIS	N-CA-CB	5.45	120.41	110.60
1	B	93	PHE	CA-C-O	-5.43	108.70	120.10
1	A	156	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	352	GLU	N-CA-CB	5.38	120.29	110.60
1	B	67	ARG	CG-CD-NE	5.38	123.09	111.80
1	B	20	THR	CA-CB-CG2	5.37	119.91	112.40
1	A	203	GLU	C-N-CA	5.36	135.09	121.70
1	B	342	GLU	CG-CD-OE2	-5.30	107.70	118.30
1	A	65	ALA	CB-CA-C	5.29	118.04	110.10
1	B	391	LEU	C-N-CA	5.28	133.40	122.30
1	B	276	ASN	C-N-CA	-5.28	111.21	122.30
1	B	173	TYR	CB-CG-CD1	5.28	124.17	121.00
1	B	342	GLU	OE1-CD-OE2	5.26	129.62	123.30
1	A	158	ARG	CD-NE-CZ	5.26	130.97	123.60
1	B	203	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	A	358	MET	CA-CB-CG	5.23	122.20	113.30
1	A	372	ALA	C-N-CA	5.23	134.78	121.70
1	B	20	THR	CB-CA-C	5.23	125.72	111.60
1	A	352	GLU	N-CA-C	-5.22	96.90	111.00
1	A	285	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	A	287	GLY	CA-C-O	5.18	129.93	120.60
1	A	328	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	222	MET	C-N-CA	5.12	134.50	121.70
1	B	186	PRO	N-CA-C	5.12	125.41	112.10
1	B	299	ASP	OD1-CG-OD2	-5.11	113.58	123.30
1	A	195	VAL	CA-CB-CG1	5.11	118.56	110.90
1	A	97	VAL	CG1-CB-CG2	-5.11	102.73	110.90
1	A	105	SER	C-N-CA	5.11	134.46	121.70
1	B	35	PRO	N-CA-CB	5.10	109.42	103.30
1	A	360	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	285	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	B	249	ARG	CA-C-N	5.07	126.34	116.20
1	B	220	GLU	OE1-CD-OE2	5.07	129.38	123.30
1	A	143	GLU	OE1-CD-OE2	-5.06	117.22	123.30
1	A	102	GLY	N-CA-C	-5.06	100.45	113.10
1	A	316	LEU	CB-CA-C	5.06	119.81	110.20
1	A	96	PRO	N-CA-CB	5.05	109.36	103.30
1	A	52	PHE	O-C-N	5.05	130.78	122.70
1	A	203	GLU	OE1-CD-OE2	-5.04	117.25	123.30

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	23	0
1	B	3027	0	2881	21	0
2	A	10	0	10	0	0
2	B	10	0	10	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	247	0	0	2	0
4	B	253	0	0	1	0
All	All	6578	0	5782	42	0

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 (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:HIS:HD2	1:A:97:VAL:H	1.31	0.79
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.78	0.66
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.77	0.65
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.79	0.63
1:B:95:HIS:HD2	1:B:97:VAL:H	1.47	0.63
1:A:135:MET:HE2	1:A:177:ILE:HG21	1.80	0.62
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.82	0.62
1:A:95:HIS:CD2	1:A:97:VAL:H	2.19	0.57
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.87	0.56
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.71	0.56
1:B:235:LEU:HD12	1:B:273:LEU:HD11	1.89	0.55
1:B:55:ASN:HA	1:B:58:ILE:O	2.08	0.54
1:A:20:THR:HG23	1:A:28:ALA:CB	2.38	0.53
1:A:84:LYS:HB2	4:A:734(A):HOH:O	2.09	0.53
1:A:135:MET:HE1	1:A:161:VAL:HG22	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:THR:HG23	1:B:28:ALA:CB	2.41	0.51
1:B:208:GLY:HA3	4:B:602(B):HOH:O	2.11	0.50
1:A:135:MET:CE	1:A:161:VAL:HG22	2.42	0.49
1:A:84:LYS:HD2	4:A:431(A):HOH:O	2.13	0.49
1:A:8:ASP:O	1:A:9:HIS:HB2	2.13	0.48
1:A:20:THR:HG23	1:A:28:ALA:HB1	1.94	0.48
1:A:135:MET:HE2	1:A:177:ILE:CG2	2.45	0.47
1:A:217:THR:HA	1:A:227:PHE:CD1	2.50	0.47
1:A:55:ASN:HA	1:A:58:ILE:O	2.15	0.47
1:B:180:GLU:HA	1:B:181:PRO:HD3	1.74	0.47
1:A:69:LYS:HE2	1:A:73:ASP:OD2	2.16	0.46
1:A:307:SER:HB3	1:B:380:ILE:HG21	1.98	0.45
1:B:256:ASP:HB3	1:B:293:TYR:HA	1.98	0.45
1:A:43:ALA:HB2	1:A:83:LEU:HD13	1.99	0.44
1:B:41:LYS:HG2	1:B:305:TRP:CD2	2.52	0.44
1:B:158:ARG:O	1:B:162:ASP:HB2	2.17	0.44
1:B:87:MET:HA	1:B:132:THR:O	2.18	0.43
1:B:35:PRO:O	1:B:39:VAL:HG23	2.19	0.43
1:A:307:SER:CB	1:B:380:ILE:HG21	2.50	0.42
1:B:278:PHE:HA	1:B:279:PRO:HD3	1.98	0.42
1:B:226:ASN:HB3	1:B:229:HIS:HB2	2.02	0.41
1:A:185:GLU:HA	1:A:186:PRO:HA	1.93	0.41
1:B:294:LYS:HA	1:B:295:PRO:HD3	1.91	0.41
1:B:16:THR:OG1	1:B:17:VAL:N	2.54	0.41
1:A:235:LEU:HD12	1:A:273:LEU:HD11	2.03	0.40
1:A:41:LYS:O	1:A:45:LEU:HG	2.21	0.40
1:A:53:HIS:O	1:A:54:ASP:C	2.60	0.40

There are no symmetry-related clashes.

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%)	368 (94%)	22 (6%)	1 (0%)	46	68
1	B	391/394 (99%)	375 (96%)	13 (3%)	3 (1%)	24	41
All	All	782/788 (99%)	743 (95%)	35 (4%)	4 (0%)	34	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU
1	B	185	GLU
1	B	3	GLN
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%)	294 (96%)	11 (4%)	42	69
1	B	305/310 (98%)	294 (96%)	11 (4%)	42	69
All	All	610/620 (98%)	588 (96%)	22 (4%)	42	69

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

Mol	Chain	Res	Type
1	A	9	HIS
1	A	20	THR
1	A	41	LYS
1	A	69	LYS
1	A	150	LEU
1	A	174	ASN
1	A	184	ASN
1	A	284	LYS
1	A	336	LYS
1	A	358	MET
1	A	359	ASN
1	B	5	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	6	PRO
1	B	20	THR
1	B	41	LYS
1	B	61	ASP
1	B	149	ASP
1	B	184	ASN
1	B	235	LEU
1	B	273	LEU
1	B	286	THR
1	B	320	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	120	HIS
1	A	184	ASN
1	A	384	GLN
1	B	75	ASN
1	B	76	GLN
1	B	95	HIS
1	B	384	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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	XYL	A	400	3	9,9,9	0.52	0	10,11,11	1.39	1 (10%)
2	XYL	B	400	3	9,9,9	0.65	0	10,11,11	1.28	1 (10%)

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	XYL	A	400	3	-	0/12/12/12	0/0/0/0
2	XYL	B	400	3	-	0/12/12/12	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	XYL	C5-C4-C3	-2.74	106.04	112.48
2	A	400	XYL	O3-C3-C2	3.17	116.73	108.75

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 [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 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.