Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:58 PM GMT

PDB ID	:	1DID
Title	:	OBSERVATIONS OF REACTION INTERMEDIATES AND THE MECHANISM OF ALDOSE-KETOSE INTERCONVERSION BY D-XYLOSE ISOMERASE
Authors	:	Collyer, C.A.; Goldberg, J.D.; Blow, D.M.
Deposited on	:	1992-06-04
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:

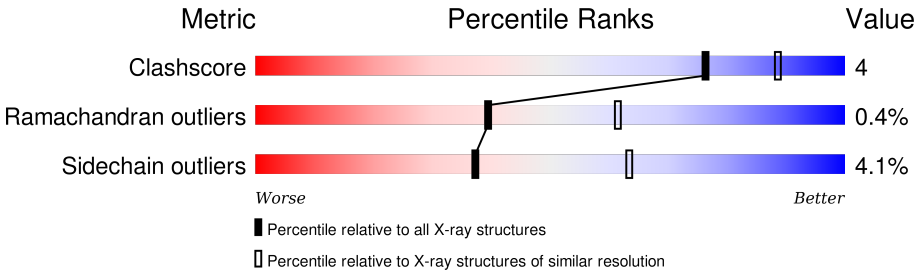
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (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	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 <=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% 25%
1	B	394	76% 21%

2 Entry composition

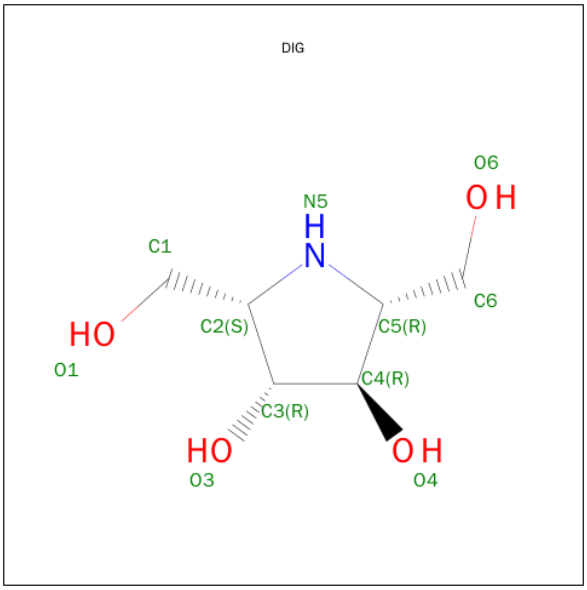
There are 4 unique types of molecules in this entry. The entry contains 6584 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2,5-DIDEOXY-2,5-IMINO-D-GLUCITOL (three-letter code: DIG) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	1	4		
2	B	1	Total	C	N	O	0	0
			11	6	1	4		

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	256	Total O 256 256	0	0
4	B	248	Total O 248 248	0	0

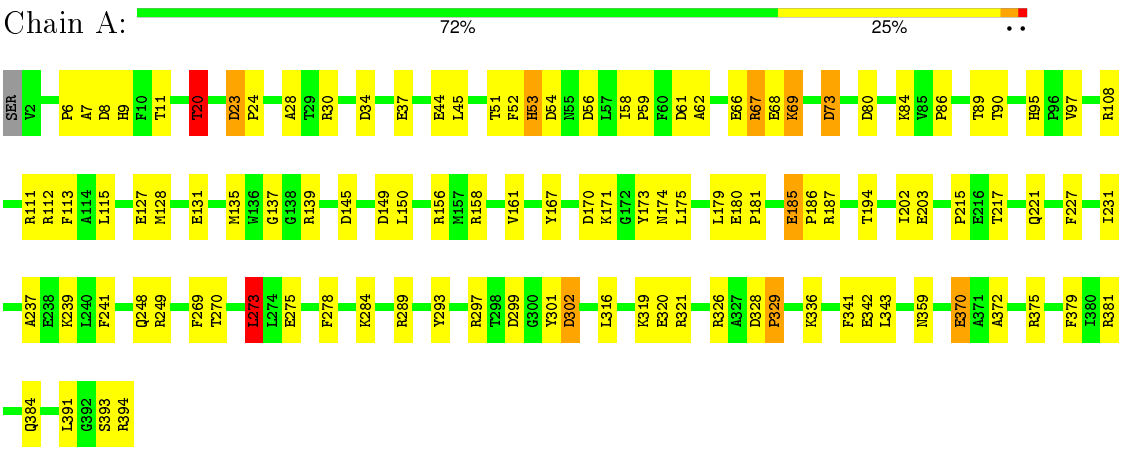
3 Residue-property plots (i)

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.

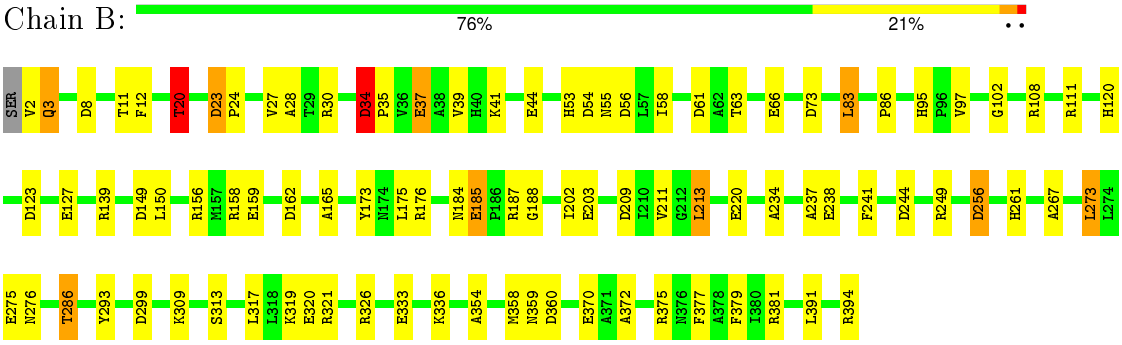
- Molecule 1: D-XYLOSE ISOMERASE

Chain A:



- Molecule 1: D-XYLOSE ISOMERASE

Chain B:



4 Data and refinement statistics (i)

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	106.10Å 106.10Å 153.30Å 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}	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6584	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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: DIG, 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	1.05	0/3101	2.07	94/4204 (2.2%)
1	B	1.05	1/3101 (0.0%)	1.94	78/4204 (1.9%)
All	All	1.05	1/6202 (0.0%)	2.00	172/8408 (2.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	GLU	CB-CG	6.21	1.64	1.52

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	394	ARG	NE-CZ-NH1	22.15	131.37	120.30
1	A	394	ARG	CD-NE-CZ	22.08	154.51	123.60
1	B	381	ARG	NE-CZ-NH2	-20.75	109.93	120.30
1	B	187	ARG	NE-CZ-NH2	-17.80	111.40	120.30
1	A	67	ARG	NE-CZ-NH1	17.03	128.81	120.30
1	A	139	ARG	NE-CZ-NH1	15.88	128.24	120.30
1	A	187	ARG	NE-CZ-NH2	-15.26	112.67	120.30
1	B	108	ARG	NE-CZ-NH1	14.35	127.47	120.30
1	A	394	ARG	NE-CZ-NH2	-13.04	113.78	120.30
1	A	139	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	B	249	ARG	NE-CZ-NH1	12.04	126.32	120.30
1	B	30	ARG	NE-CZ-NH1	11.67	126.14	120.30
1	A	111	ARG	NE-CZ-NH1	11.53	126.07	120.30
1	B	156	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	B	375	ARG	NE-CZ-NH2	-11.27	114.67	120.30
1	B	34	ASP	CB-CG-OD2	-10.86	108.53	118.30
1	A	299	ASP	CB-CG-OD1	10.53	127.78	118.30
1	A	8	ASP	CB-CG-OD2	10.50	127.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	381	ARG	NE-CZ-NH1	10.43	125.51	120.30
1	A	375	ARG	NE-CZ-NH2	-10.17	115.22	120.30
1	A	67	ARG	NE-CZ-NH2	-10.13	115.23	120.30
1	B	111	ARG	NE-CZ-NH2	-10.05	115.27	120.30
1	B	111	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	A	149	ASP	CB-CG-OD1	9.76	127.09	118.30
1	B	394	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	A	381	ARG	NE-CZ-NH1	9.65	125.13	120.30
1	B	34	ASP	CB-CG-OD1	9.44	126.80	118.30
1	A	34	ASP	CB-CG-OD2	9.20	126.58	118.30
1	A	23	ASP	CB-CG-OD1	9.04	126.44	118.30
1	A	342	GLU	N-CA-CB	8.97	126.74	110.60
1	A	68	GLU	OE1-CD-OE2	8.86	133.93	123.30
1	B	321	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	A	108	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	B	299	ASP	CB-CG-OD1	8.71	126.14	118.30
1	A	51	THR	CA-CB-CG2	8.40	124.16	112.40
1	A	187	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	B	273	LEU	CA-CB-CG	8.16	134.07	115.30
1	A	342	GLU	CA-CB-CG	8.15	131.33	113.40
1	A	6	PRO	C-N-CA	8.13	142.04	121.70
1	A	289	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	A	73	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	A	326	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	A	113	PHE	CB-CG-CD2	-7.65	115.44	120.80
1	B	20	THR	CA-CB-CG2	7.59	123.03	112.40
1	B	139	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	241	PHE	CB-CG-CD1	7.53	126.07	120.80
1	B	286	THR	N-CA-CB	-7.50	96.06	110.30
1	B	256	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	A	342	GLU	OE1-CD-OE2	7.45	132.24	123.30
1	B	333	GLU	CA-CB-CG	7.31	129.47	113.40
1	B	23	ASP	CB-CA-C	7.24	124.88	110.40
1	A	269	PHE	CB-CG-CD1	-7.22	115.75	120.80
1	A	67	ARG	CD-NE-CZ	7.18	133.66	123.60
1	B	187	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	B	53	HIS	N-CA-CB	7.11	123.39	110.60
1	B	20	THR	N-CA-CB	-7.08	96.84	110.30
1	B	156	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	B	238	GLU	CA-CB-CG	-7.06	97.86	113.40
1	A	297	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	112	ARG	CD-NE-CZ	6.98	133.37	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	156	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	321	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	301	TYR	CB-CG-CD2	-6.91	116.85	121.00
1	A	145	ASP	CB-CG-OD1	6.84	124.46	118.30
1	A	149	ASP	N-CA-CB	6.82	122.87	110.60
1	A	273	LEU	CA-CB-CG	6.79	130.91	115.30
1	B	213	LEU	CA-CB-CG	6.78	130.90	115.30
1	A	381	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	B	372	ALA	O-C-N	-6.77	111.88	122.70
1	B	37	GLU	CA-CB-CG	6.75	128.25	113.40
1	A	237	ALA	C-N-CA	6.73	138.53	121.70
1	A	370	GLU	CG-CD-OE2	6.68	131.67	118.30
1	A	37	GLU	OE1-CD-OE2	6.65	131.28	123.30
1	B	377	PHE	CB-CG-CD1	-6.64	116.15	120.80
1	A	249	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	B	360	ASP	CB-CG-OD2	6.44	124.10	118.30
1	A	112	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	173	TYR	CB-CG-CD1	6.25	124.75	121.00
1	A	137	GLY	C-N-CA	6.23	135.39	122.30
1	B	370	GLU	OE1-CD-OE2	6.22	130.77	123.30
1	A	54	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	370	GLU	CG-CD-OE1	-6.20	105.91	118.30
1	B	108	ARG	CD-NE-CZ	6.19	132.27	123.60
1	B	73	ASP	CA-CB-CG	6.13	126.88	113.40
1	B	120	HIS	CA-CB-CG	-6.11	103.21	113.60
1	B	158	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	53	HIS	N-CA-CB	6.03	121.45	110.60
1	A	175	LEU	CA-CB-CG	6.03	129.16	115.30
1	A	321	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	203	GLU	CG-CD-OE2	6.01	130.32	118.30
1	A	56	ASP	CB-CG-OD2	5.97	123.68	118.30
1	A	170	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	B	320	GLU	CA-CB-CG	5.96	126.50	113.40
1	B	256	ASP	CB-CG-OD1	5.94	123.65	118.30
1	B	83	LEU	CA-CB-CG	5.90	128.88	115.30
1	A	61	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	173	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	B	8	ASP	CB-CG-OD2	5.89	123.61	118.30
1	A	115	LEU	CB-CA-C	5.88	121.37	110.20
1	A	167	TYR	CB-CG-CD1	-5.87	117.48	121.00
1	B	173	TYR	CB-CG-CD1	5.87	124.52	121.00
1	A	7	ALA	C-N-CA	5.86	136.34	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	220	GLU	OE1-CD-OE2	5.85	130.31	123.30
1	B	359	ASN	CB-CA-C	5.79	121.97	110.40
1	A	320	GLU	CG-CD-OE2	5.76	129.82	118.30
1	A	342	GLU	CB-CA-C	-5.73	98.93	110.40
1	B	391	LEU	C-N-CA	5.71	134.28	122.30
1	B	244	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	123	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	391	LEU	C-N-CA	5.68	134.22	122.30
1	B	370	GLU	CG-CD-OE1	-5.67	106.95	118.30
1	A	320	GLU	CA-CB-CG	5.67	125.87	113.40
1	A	302	ASP	CB-CG-OD2	-5.64	113.23	118.30
1	A	379	PHE	CB-CG-CD2	-5.62	116.86	120.80
1	A	131	GLU	CG-CD-OE1	5.59	129.49	118.30
1	A	30	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	149	ASP	N-CA-C	-5.57	95.97	111.00
1	A	343	LEU	C-N-CA	5.56	133.98	122.30
1	A	111	ARG	NH1-CZ-NH2	-5.55	113.30	119.40
1	B	249	ARG	CA-C-N	5.53	127.27	116.20
1	A	45	LEU	CA-C-N	5.53	127.25	116.20
1	A	52	PHE	CB-CG-CD2	-5.49	116.95	120.80
1	A	128	MET	O-C-N	-5.49	113.86	123.20
1	B	237	ALA	C-N-CA	5.48	135.39	121.70
1	B	267	ALA	N-CA-CB	5.47	117.76	110.10
1	A	20	THR	N-CA-CB	-5.46	99.93	110.30
1	A	44	GLU	CA-CB-CG	5.44	125.38	113.40
1	B	44	GLU	CA-CB-CG	5.44	125.37	113.40
1	B	165	ALA	CB-CA-C	5.43	118.24	110.10
1	B	150	LEU	CB-CA-C	5.41	120.49	110.20
1	B	209	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	320	GLU	CG-CD-OE1	-5.37	107.56	118.30
1	B	187	ARG	CD-NE-CZ	5.37	131.12	123.60
1	A	34	ASP	OD1-CG-OD2	-5.37	113.11	123.30
1	B	44	GLU	CG-CD-OE1	-5.36	107.58	118.30
1	A	316	LEU	CB-CA-C	5.36	120.37	110.20
1	A	297	ARG	O-C-N	-5.35	114.14	122.70
1	B	326	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	159	GLU	CA-CB-CG	5.32	125.10	113.40
1	B	56	ASP	CB-CG-OD1	5.32	123.08	118.30
1	B	249	ARG	CD-NE-CZ	5.32	131.05	123.60
1	A	30	ARG	CD-NE-CZ	5.32	131.04	123.60
1	A	194	THR	CA-CB-CG2	5.31	119.83	112.40
1	B	379	PHE	CB-CG-CD2	-5.31	117.08	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	341	PHE	CB-CG-CD1	-5.29	117.10	120.80
1	A	391	LEU	CA-CB-CG	5.29	127.46	115.30
1	B	108	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	23	ASP	CB-CA-C	5.29	120.97	110.40
1	A	127	GLU	OE1-CD-OE2	5.29	129.64	123.30
1	A	173	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	A	66	GLU	CG-CD-OE2	5.22	128.75	118.30
1	B	175	LEU	CA-CB-CG	5.20	127.27	115.30
1	A	329	PRO	C-N-CA	5.20	134.70	121.70
1	B	241	PHE	CB-CG-CD2	-5.18	117.18	120.80
1	A	301	TYR	CG-CD2-CE2	-5.14	117.19	121.30
1	A	270	THR	CA-CB-CG2	5.13	119.58	112.40
1	A	372	ALA	O-C-N	-5.11	114.52	122.70
1	B	12	PHE	CB-CG-CD1	-5.11	117.22	120.80
1	B	102	GLY	N-CA-C	-5.11	100.33	113.10
1	B	188	GLY	O-C-N	-5.11	114.53	122.70
1	A	293	TYR	CB-CG-CD2	5.10	124.06	121.00
1	A	156	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	158	ARG	CD-NE-CZ	5.08	130.72	123.60
1	B	54	ASP	O-C-N	-5.08	114.57	122.70
1	A	80	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	B	372	ALA	CB-CA-C	5.05	117.68	110.10
1	B	185	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	A	203	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	B	127	GLU	CA-CB-CG	5.03	124.48	113.40
1	B	27	VAL	CA-CB-CG2	5.03	118.44	110.90
1	B	162	ASP	CB-CA-C	5.02	120.43	110.40
1	B	234	ALA	N-CA-CB	5.01	117.11	110.10

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	2880	27	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3027	0	2882	19	1
2	A	11	0	11	0	0
2	B	11	0	11	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	256	0	0	4	0
4	B	248	0	0	1	1
All	All	6584	0	5784	45	2

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 (45) 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:95:HIS:HD2	1:B:97:VAL:H	1.41	0.68
1:A:95:HIS:HD2	1:A:97:VAL:H	1.39	0.68
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.79	0.64
1:A:23:ASP:HB2	1:A:24:PRO:HD2	1.80	0.62
1:A:69:LYS:HE2	1:A:73:ASP:OD2	2.00	0.62
1:A:59:PRO:HG2	1:A:62:ALA:HB2	1.84	0.59
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.86	0.57
1:B:23:ASP:HB2	1:B:24:PRO:HD2	1.88	0.55
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.88	0.54
1:B:55:ASN:HA	1:B:58:ILE:O	2.08	0.54
1:B:256:ASP:HB3	1:B:293:TYR:HA	1.91	0.53
1:A:95:HIS:CD2	1:A:97:VAL:H	2.23	0.52
1:A:20:THR:HG23	1:A:28:ALA:CB	2.40	0.52
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.93	0.51
1:B:354:ALA:O	1:B:358:MET:HG3	2.12	0.50
1:B:20:THR:HG23	1:B:28:ALA:CB	2.41	0.50
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.95	0.49
1:A:84:LYS:HD2	4:A:422:HOH:O	2.13	0.48
1:A:202:ILE:HG21	1:A:239:LYS:HE3	1.96	0.48
1:B:2:VAL:HG23	1:B:3:GLN:H	1.79	0.47
1:A:215:PRO:HG2	1:A:231:ILE:HG22	1.96	0.47
1:A:135:MET:CE	1:A:161:VAL:HG22	2.44	0.47
1:A:20:THR:HG23	1:A:28:ALA:HB2	1.96	0.46
1:A:185:GLU:HA	1:A:186:PRO:HA	1.75	0.45
1:A:58:ILE:HG21	1:A:67:ARG:HG3	1.99	0.45
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.80	0.43
1:B:20:THR:HG22	4:B:563:HOH:O	2.17	0.43
1:A:84:LYS:HB2	4:A:627:HOH:O	2.17	0.43
1:B:309:LYS:HB3	1:B:309:LYS:HE2	1.79	0.43
1:A:135:MET:HE3	1:A:161:VAL:HG22	2.01	0.43
1:A:217:THR:HA	1:A:227:PHE:CD1	2.55	0.42
1:A:179:LEU:HD22	4:A:442:HOH:O	2.20	0.41
1:A:275:GLU:HG3	1:A:319:LYS:HG3	2.01	0.41
1:A:273:LEU:HD21	1:A:278:PHE:CE1	2.55	0.41
1:A:384:GLN:NE2	1:B:261:HIS:NE2	2.67	0.41
1:B:23:ASP:CB	1:B:24:PRO:HD2	2.50	0.41
1:B:202:ILE:HG12	1:B:211:VAL:HG12	2.01	0.41
1:A:20:THR:HB	4:A:535:HOH:O	2.21	0.41
1:B:313:SER:O	1:B:317:LEU:HG	2.21	0.41
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.55	0.41
1:A:58:ILE:CG2	1:A:67:ARG:HG3	2.51	0.40
1:B:63:THR:HG23	1:B:66:GLU:OE2	2.21	0.40
1:A:180:GLU:HA	1:A:181:PRO:HD3	1.88	0.40
1:B:34:ASP:HA	1:B:35:PRO:HD3	1.83	0.40

All (2) 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)
4:B:515:HOH:O	4:B:580:HOH:O[4_555]	1.92	0.28
1:A:69:LYS:NZ	1:B:276:ASN:O[6_665]	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%)	373 (95%)	17 (4%)	1 (0%)	46 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	391/394 (99%)	380 (97%)	9 (2%)	2 (0%)	34 55
All	All	782/788 (99%)	753 (96%)	26 (3%)	3 (0%)	39 61

All (3) Ramachandran outliers are listed below:

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

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%)	33 57
1	B	305/310 (98%)	294 (96%)	11 (4%)	42 69
All	All	610/620 (98%)	585 (96%)	25 (4%)	37 63

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

Mol	Chain	Res	Type
1	A	9	HIS
1	A	20	THR
1	A	69	LYS
1	A	90	THR
1	A	150	LEU
1	A	171	LYS
1	A	174	ASN
1	A	273	LEU
1	A	284	LYS
1	A	302	ASP
1	A	336	LYS
1	A	359	ASN
1	A	370	GLU

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Mol	Chain	Res	Type
1	A	393	SER
1	B	20	THR
1	B	34	ASP
1	B	37	GLU
1	B	41	LYS
1	B	61	ASP
1	B	176	ARG
1	B	184	ASN
1	B	213	LEU
1	B	273	LEU
1	B	286	THR
1	B	336	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	95	HIS
1	A	174	ASN
1	A	221	GLN
1	A	384	GLN
1	B	75	ASN
1	B	76	GLN
1	B	95	HIS
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 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	DIG	A	400	3	11,11,11	2.10	4 (36%)	8,15,15	1.98	4 (50%)
2	DIG	B	400	3	11,11,11	2.68	5 (45%)	8,15,15	1.85	3 (37%)

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	DIG	A	400	3	-	0/4/20/20	0/1/1/1
2	DIG	B	400	3	-	0/4/20/20	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	DIG	C4-C5	-5.34	1.49	1.53
2	B	400	DIG	C2-N5	-4.91	1.40	1.48
2	B	400	DIG	O4-C4	-3.20	1.35	1.43
2	A	400	DIG	O1-C1	-2.90	1.29	1.42
2	B	400	DIG	O1-C1	-2.52	1.31	1.42
2	B	400	DIG	C5-N5	-2.52	1.44	1.48
2	A	400	DIG	C5-N5	-2.46	1.44	1.48
2	A	400	DIG	C2-N5	-2.15	1.45	1.48
2	A	400	DIG	C3-C2	4.37	1.57	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	DIG	C1-C2-C3	-2.47	109.79	114.10
2	A	400	DIG	C3-C4-C5	2.18	106.81	103.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	400	DIG	O1-C1-C2	2.21	117.05	111.12
2	B	400	DIG	C3-C4-C5	2.46	107.27	103.17
2	A	400	DIG	O6-C6-C5	2.77	118.53	111.12
2	B	400	DIG	O6-C6-C5	3.38	120.17	111.12
2	A	400	DIG	O1-C1-C2	3.51	120.51	111.12

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.