Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 04:29 AM EST

PDB ID	:	1XLH
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 ⓘ 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 ⓘ) were used in the production of this report:

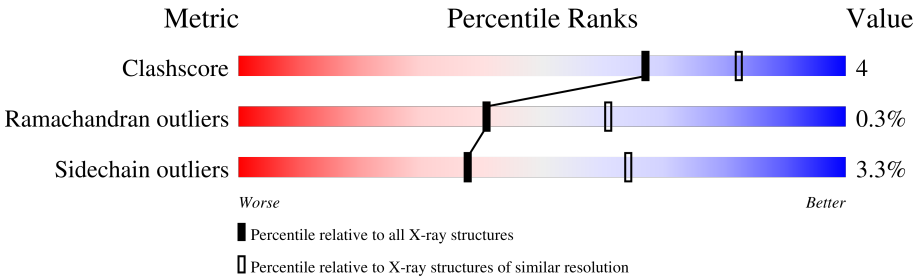
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	75% 21% .
1	B	394	76% 20% . .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6602 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 ALUMINUM ION (three-letter code: AL) (formula: Al).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Al	0	0
			1	1		
2	B	1	Total	Al	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	270	Total	O	0	0
			270	270		
3	B	276	Total	O	0	0
			276	276		

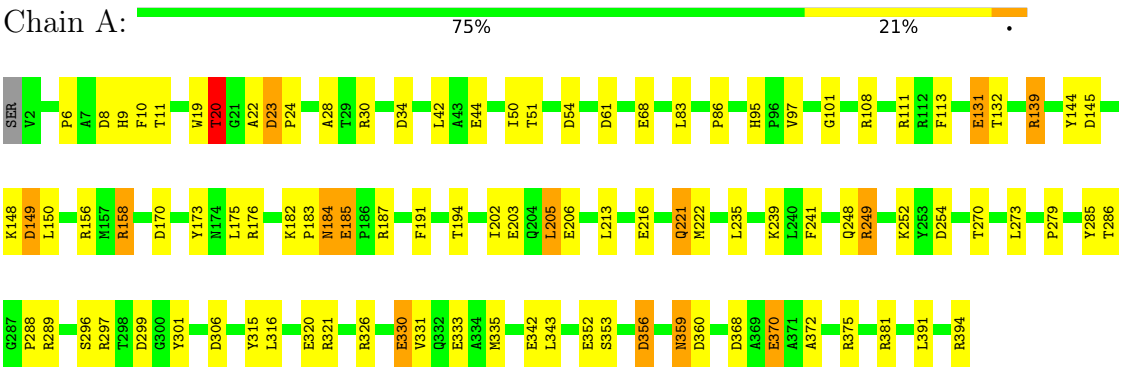
3 Residue-property plots (i)

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.

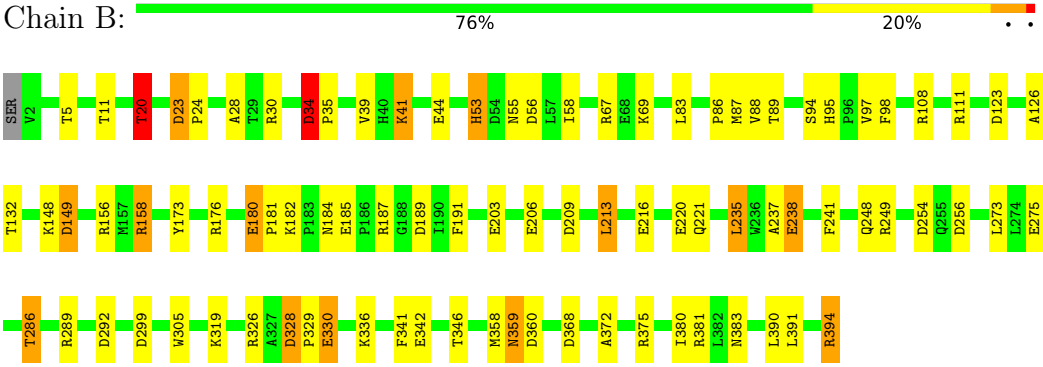
• Molecule 1: D-XYLOSE ISOMERASE

Chain A:



• Molecule 1: D-XYLOSE ISOMERASE

Chain B:



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	105.80Å 105.80Å 153.50Å 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}	0.154 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6602	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: AL

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	2.04	101/4204 (2.4%)
1	B	1.07	2/3101 (0.1%)	2.06	82/4204 (2.0%)
All	All	1.06	2/6202 (0.0%)	2.05	183/8408 (2.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	254	ASP	CA-CB	-5.55	1.41	1.53
1	B	220	GLU	CD-OE1	-5.13	1.20	1.25

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	394	ARG	CD-NE-CZ	26.41	160.57	123.60
1	B	187	ARG	NE-CZ-NH2	-22.70	108.95	120.30
1	B	158	ARG	NE-CZ-NH2	-21.83	109.39	120.30
1	B	394	ARG	NE-CZ-NH2	-20.09	110.26	120.30
1	B	381	ARG	NE-CZ-NH2	-17.75	111.42	120.30
1	B	158	ARG	NE-CZ-NH1	17.65	129.12	120.30
1	A	394	ARG	NE-CZ-NH1	16.01	128.31	120.30
1	B	30	ARG	NE-CZ-NH1	15.68	128.14	120.30
1	A	289	ARG	CD-NE-CZ	14.03	143.25	123.60
1	B	187	ARG	NE-CZ-NH1	14.01	127.31	120.30
1	B	111	ARG	NE-CZ-NH1	13.82	127.21	120.30
1	A	30	ARG	NE-CZ-NH2	-13.21	113.70	120.30
1	B	156	ARG	NE-CZ-NH2	-12.80	113.90	120.30
1	A	359	ASN	CA-CB-CG	12.64	141.22	113.40
1	A	301	TYR	CB-CG-CD2	-12.32	113.61	121.00
1	B	34	ASP	CB-CG-OD2	12.32	129.38	118.30
1	A	30	ARG	NE-CZ-NH1	12.19	126.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	111	ARG	NE-CZ-NH2	-12.06	114.27	120.30
1	B	254	ASP	CA-CB-CG	11.60	138.92	113.40
1	B	299	ASP	CB-CG-OD1	11.11	128.30	118.30
1	B	249	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	A	375	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	A	44	GLU	CA-CB-CG	10.53	136.56	113.40
1	A	156	ARG	NE-CZ-NH1	10.35	125.47	120.30
1	A	187	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	B	375	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	B	108	ARG	NE-CZ-NH1	10.16	125.38	120.30
1	B	156	ARG	NE-CZ-NH1	10.10	125.35	120.30
1	A	375	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	B	108	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	A	111	ARG	NE-CZ-NH1	9.99	125.29	120.30
1	A	176	ARG	NE-CZ-NH1	9.93	125.26	120.30
1	B	176	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	B	149	ASP	CB-CG-OD1	9.55	126.90	118.30
1	A	23	ASP	CB-CG-OD1	9.49	126.84	118.30
1	B	30	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	B	256	ASP	CB-CG-OD2	-9.30	109.92	118.30
1	A	254	ASP	CA-CB-CG	9.09	133.41	113.40
1	A	299	ASP	CB-CG-OD1	8.86	126.27	118.30
1	B	131	GLU	OE1-CD-OE2	-8.77	112.78	123.30
1	B	56	ASP	CB-CG-OD2	8.73	126.16	118.30
1	B	123	ASP	CB-CG-OD2	8.69	126.12	118.30
1	A	6	PRO	C-N-CA	8.60	143.19	121.70
1	A	326	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	149	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	A	394	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	B	44	GLU	CA-CB-CG	8.16	131.35	113.40
1	A	241	PHE	CB-CG-CD1	8.12	126.49	120.80
1	B	131	GLU	CA-CB-CG	8.08	131.17	113.40
1	A	156	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A	306	ASP	CB-CG-OD2	8.00	125.50	118.30
1	A	34	ASP	CB-CG-OD1	7.99	125.49	118.30
1	A	149	ASP	CB-CG-OD1	7.92	125.43	118.30
1	A	51	THR	CA-CB-CG2	7.83	123.36	112.40
1	A	6	PRO	O-C-N	-7.83	110.17	122.70
1	B	20	THR	N-CA-CB	-7.77	95.53	110.30
1	B	372	ALA	CB-CA-C	7.67	121.61	110.10
1	A	131	GLU	CB-CG-CD	7.65	134.85	114.20
1	A	68	GLU	OE1-CD-OE2	7.47	132.27	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	326	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	B	203	GLU	CG-CD-OE2	7.35	133.01	118.30
1	A	297	ARG	CD-NE-CZ	7.32	133.85	123.60
1	B	360	ASP	CB-CG-OD2	7.27	124.84	118.30
1	B	328	ASP	CB-CG-OD1	7.23	124.81	118.30
1	B	23	ASP	CB-CA-C	7.17	124.75	110.40
1	A	139	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	203	GLU	OE1-CD-OE2	-7.12	114.76	123.30
1	A	333	GLU	CA-CB-CG	7.04	128.88	113.40
1	B	131	GLU	CG-CD-OE2	6.95	132.20	118.30
1	B	286	THR	N-CA-CB	-6.91	97.17	110.30
1	A	216	GLU	OE1-CD-OE2	6.87	131.55	123.30
1	A	19	TRP	C-N-CA	6.83	138.78	121.70
1	A	320	GLU	CA-CB-CG	6.78	128.32	113.40
1	B	20	THR	CA-CB-CG2	6.78	121.89	112.40
1	B	394	ARG	NH1-CZ-NH2	6.77	126.84	119.40
1	A	203	GLU	CG-CD-OE2	6.74	131.78	118.30
1	B	98	PHE	CB-CG-CD2	-6.69	116.12	120.80
1	B	358	MET	CG-SD-CE	6.66	110.85	100.20
1	B	289	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	B	330	GLU	CA-CB-CG	6.63	127.99	113.40
1	A	285	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	B	209	ASP	CB-CG-OD2	6.63	124.27	118.30
1	B	127	GLU	CA-CB-CG	6.61	127.93	113.40
1	B	330	GLU	CG-CD-OE1	-6.58	105.14	118.30
1	B	5	THR	CA-CB-CG2	6.53	121.53	112.40
1	A	249	ARG	CD-NE-CZ	6.52	132.72	123.60
1	A	187	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	249	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	158	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	297	ARG	CG-CD-NE	6.48	125.41	111.80
1	B	368	ASP	CB-CG-OD1	6.48	124.13	118.30
1	A	270	THR	CA-CB-CG2	6.46	121.45	112.40
1	A	381	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	111	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	289	ARG	CA-CB-CG	6.36	127.39	113.40
1	A	326	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	213	LEU	CA-CB-CG	6.30	129.80	115.30
1	A	356	ASP	CB-CG-OD2	6.26	123.94	118.30
1	B	342	GLU	CG-CD-OE2	-6.23	105.83	118.30
1	A	22	ALA	CB-CA-C	6.21	119.41	110.10
1	A	360	ASP	CB-CG-OD2	6.20	123.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	320	GLU	OE1-CD-OE2	-6.19	115.87	123.30
1	B	189	ASP	CB-CG-OD1	-6.16	112.76	118.30
1	A	173	TYR	CB-CG-CD1	6.14	124.69	121.00
1	B	126	ALA	CB-CA-C	6.01	119.12	110.10
1	B	216	GLU	OE1-CD-OE2	5.98	130.47	123.30
1	A	139	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	149	ASP	N-CA-C	-5.94	94.97	111.00
1	A	370	GLU	CG-CD-OE1	-5.89	106.52	118.30
1	A	213	LEU	CA-CB-CG	5.88	128.83	115.30
1	B	53	HIS	N-CA-CB	5.86	121.16	110.60
1	B	149	ASP	N-CA-C	-5.82	95.30	111.00
1	B	203	GLU	C-N-CA	5.81	136.22	121.70
1	B	381	ARG	NH1-CZ-NH2	5.80	125.78	119.40
1	A	185	GLU	OE1-CD-OE2	-5.80	116.34	123.30
1	A	320	GLU	CG-CD-OE2	5.79	129.87	118.30
1	A	321	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	B	67	ARG	CG-CD-NE	5.77	123.92	111.80
1	A	368	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	333	GLU	CG-CD-OE1	5.71	129.71	118.30
1	A	206	GLU	N-CA-CB	5.70	120.86	110.60
1	A	54	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	343	LEU	C-N-CA	5.68	134.23	122.30
1	B	56	ASP	N-CA-CB	5.67	120.81	110.60
1	A	20	THR	CA-CB-CG2	5.67	120.34	112.40
1	A	352	GLU	OE1-CD-OE2	-5.66	116.51	123.30
1	A	170	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	254	ASP	N-CA-CB	5.62	120.72	110.60
1	A	108	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	175	LEU	CB-CA-C	-5.59	99.59	110.20
1	B	123	ASP	OD1-CG-OD2	-5.57	112.72	123.30
1	A	372	ALA	O-C-N	-5.55	113.81	122.70
1	A	286	THR	CA-CB-OG1	-5.54	97.37	109.00
1	B	241	PHE	CB-CG-CD1	5.54	124.67	120.80
1	A	194	THR	CA-CB-CG2	5.53	120.14	112.40
1	B	372	ALA	O-C-N	-5.52	113.86	122.70
1	A	205	LEU	CA-CB-CG	5.44	127.80	115.30
1	A	330	GLU	CG-CD-OE1	-5.41	107.48	118.30
1	B	342	GLU	OE1-CD-OE2	5.41	129.79	123.30
1	A	111	ARG	CD-NE-CZ	5.40	131.16	123.60
1	A	352	GLU	CG-CD-OE2	5.39	129.09	118.30
1	B	292	ASP	CB-CG-OD1	5.39	123.16	118.30
1	A	10	PHE	CB-CG-CD2	-5.38	117.03	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	145	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	241	PHE	CB-CG-CD2	-5.37	117.04	120.80
1	A	144	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	A	342	GLU	CG-CD-OE2	-5.36	107.59	118.30
1	A	286	THR	OG1-CB-CG2	5.35	122.30	110.00
1	A	316	LEU	CB-CA-C	5.34	120.34	110.20
1	A	149	ASP	N-CA-CB	5.32	120.18	110.60
1	A	315	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	B	180	GLU	CG-CD-OE2	-5.30	107.69	118.30
1	A	289	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	173	TYR	CB-CG-CD1	5.28	124.17	121.00
1	B	44	GLU	CG-CD-OE1	-5.27	107.76	118.30
1	A	113	PHE	CB-CG-CD2	-5.26	117.11	120.80
1	B	390	LEU	O-C-N	-5.25	114.30	122.70
1	A	150	LEU	CB-CA-C	5.24	120.16	110.20
1	B	391	LEU	C-N-CA	5.24	133.30	122.30
1	B	88	VAL	CG1-CB-CG2	-5.23	102.53	110.90
1	B	346	THR	CA-CB-OG1	-5.23	98.02	109.00
1	B	249	ARG	CD-NE-CZ	5.22	130.91	123.60
1	A	241	PHE	CB-CG-CD2	-5.22	117.15	120.80
1	A	279	PRO	O-C-N	-5.22	114.35	122.70
1	A	83	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	301	TYR	CG-CD1-CE1	-5.21	117.14	121.30
1	A	61	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	285	TYR	CB-CG-CD1	5.19	124.11	121.00
1	A	391	LEU	C-N-CA	5.18	133.18	122.30
1	B	108	ARG	CD-NE-CZ	5.18	130.85	123.60
1	B	128	MET	CG-SD-CE	-5.17	91.92	100.20
1	B	203	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	A	222	MET	C-N-CA	5.15	134.58	121.70
1	A	288	PRO	O-C-N	5.15	130.94	122.70
1	B	176	ARG	CB-CG-CD	5.13	124.94	111.60
1	A	352	GLU	N-CA-CB	5.13	119.83	110.60
1	B	203	GLU	CA-C-N	5.11	128.44	117.20
1	B	20	THR	CB-CA-C	5.09	125.35	111.60
1	A	173	TYR	CB-CG-CD2	-5.09	117.95	121.00
1	A	221	GLN	C-N-CA	5.08	134.39	121.70
1	B	206	GLU	CG-CD-OE2	-5.07	108.16	118.30
1	B	238	GLU	CG-CD-OE1	-5.02	108.26	118.30
1	B	383	ASN	CB-CG-OD1	-5.00	111.59	121.60

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	22	0
1	B	3027	0	2882	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	270	0	0	0	1
3	B	276	0	0	1	1
All	All	6602	0	5762	46	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 (46) 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	1.37	0.70
1:B:95:HIS:HD2	1:B:97:VAL:H	1.40	0.68
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.74	0.68
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.76	0.68
1:B:235:LEU:HD12	1:B:273:LEU:HD21	1.79	0.65
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.84	0.59
1:A:235:LEU:HD12	1:A:273:LEU:HD21	1.84	0.58
1:B:23:ASP:HB2	1:B:24:PRO:HD2	1.88	0.55
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.73	0.53
1:B:182:LYS:HE2	1:B:184:ASN:O	2.09	0.53
1:A:296:SER:H	1:B:380:ILE:HD11	1.75	0.52
1:A:202:ILE:HG21	1:A:239:LYS:HE3	1.92	0.51
1:A:182:LYS:HE2	1:A:184:ASN:O	2.11	0.51
1:A:20:THR:HG23	1:A:28:ALA:CB	2.43	0.49
1:B:148:LYS:HG3	1:B:191:PHE:HZ	1.77	0.49
1:B:158:ARG:HD2	3:B:469(B):HOH:O	2.13	0.48
1:A:131:GLU:HG3	1:A:132:THR:N	2.28	0.47
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LYS:HG3	1:A:183:PRO:HD2	1.95	0.46
1:B:20:THR:HG23	1:B:28:ALA:CB	2.45	0.46
1:A:23:ASP:HB2	1:A:24:PRO:CD	2.46	0.46
1:A:42:LEU:HD12	1:A:50:ILE:HD12	1.99	0.45
1:B:35:PRO:O	1:B:39:VAL:HG23	2.15	0.45
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.81	0.45
1:A:296:SER:N	1:B:380:ILE:HD11	2.32	0.45
1:B:328:ASP:HA	1:B:329:PRO:HD3	1.82	0.45
1:A:101:GLY:HA2	1:A:139:ARG:HB2	1.99	0.45
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.98	0.44
1:A:95:HIS:CD2	1:A:97:VAL:H	2.27	0.44
1:A:353:SER:H	1:A:356:ASP:HB2	1.82	0.44
1:A:8:ASP:O	1:A:9:HIS:HB2	2.18	0.43
1:B:280:ASN:OD1	1:B:341:PHE:HA	2.18	0.43
1:B:41:LYS:HG2	1:B:305:TRP:CE2	2.54	0.42
1:B:278:PHE:HA	1:B:279:PRO:HD3	1.90	0.42
1:A:158:ARG:HG3	1:A:205:LEU:HD23	2.01	0.41
1:B:180:GLU:HA	1:B:181:PRO:HD3	1.77	0.41
1:B:53:HIS:CD2	1:B:89:THR:HG23	2.55	0.41
1:B:359:ASN:C	1:B:359:ASN:HD22	2.23	0.41
1:A:331:VAL:O	1:A:335:MET:HG3	2.21	0.41
1:B:221:GLN:HE21	1:B:248:GLN:HB3	1.86	0.41
1:A:20:THR:HG23	1:A:28:ALA:HB2	2.01	0.41
1:B:34:ASP:HA	1:B:35:PRO:HD3	1.81	0.41
1:B:55:ASN:HA	1:B:58:ILE:O	2.21	0.41
1:B:237:ALA:O	1:B:238:GLU:HB2	2.21	0.40
1:B:87:MET:HA	1:B:132:THR:O	2.22	0.40
1:A:249:ARG:O	1:A:252:LYS:HE3	2.21	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)
3:B:573(B):HOH:O	3:B:614(B):HOH:O[4_555]	2.01	0.19
3:A:473(A):HOH:O	3:A:597(A):HOH:O[4_555]	2.18	0.02

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%)	375 (96%)	15 (4%)	1 (0%)	41 61
1	B	391/394 (99%)	376 (96%)	14 (4%)	1 (0%)	41 61
All	All	782/788 (99%)	751 (96%)	29 (4%)	2 (0%)	41 61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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%)	299 (98%)	6 (2%)	55 79
1	B	305/310 (98%)	291 (95%)	14 (5%)	27 50
All	All	610/620 (98%)	590 (97%)	20 (3%)	38 64

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	149	ASP
1	A	184	ASN
1	A	330	GLU

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Mol	Chain	Res	Type
1	A	359	ASN
1	A	370	GLU
1	B	20	THR
1	B	34	ASP
1	B	41	LYS
1	B	69	LYS
1	B	94	SER
1	B	131	GLU
1	B	149	ASP
1	B	213	LEU
1	B	235	LEU
1	B	286	THR
1	B	330	GLU
1	B	336	LYS
1	B	359	ASN
1	B	394	ARG

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

Mol	Chain	Res	Type
1	A	75	ASN
1	A	95	HIS
1	A	184	ASN
1	A	221	GLN
1	A	384	GLN
1	B	9	HIS
1	B	95	HIS
1	B	221	GLN
1	B	359	ASN
1	B	384	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.