



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:57 PM UTC

PDB ID : 1XIG / pdb_00001xig
Title : MODES OF BINDING SUBSTRATES AND THEIR ANALOGUES TO THE
ENZYME D-XYLOSE ISOMERASE
Authors : Carrell, H.L.; Glusker, J.P.
Deposited on : 1994-03-07
Resolution : 1.70 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

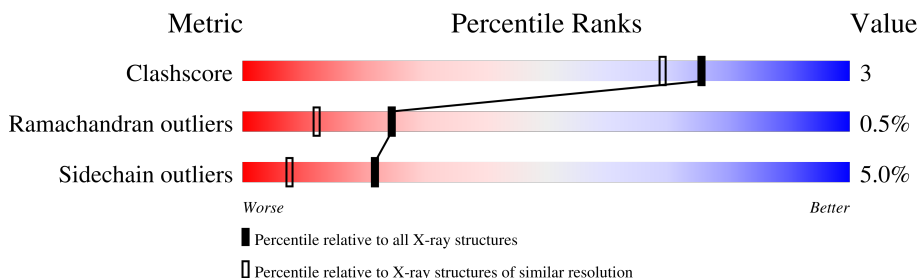
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	388	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3339 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.

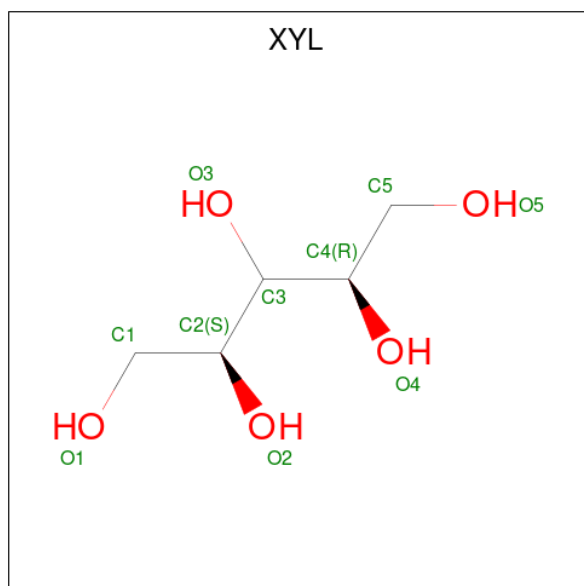
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	3031	1906	545	572	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	GLN	ARG	conflict	UNP P24300

- Molecule 2 is Xylitol (CCD ID: XYL) (formula: C₅H₁₂O₅).



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

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	296	Total 296	O 296	0	0

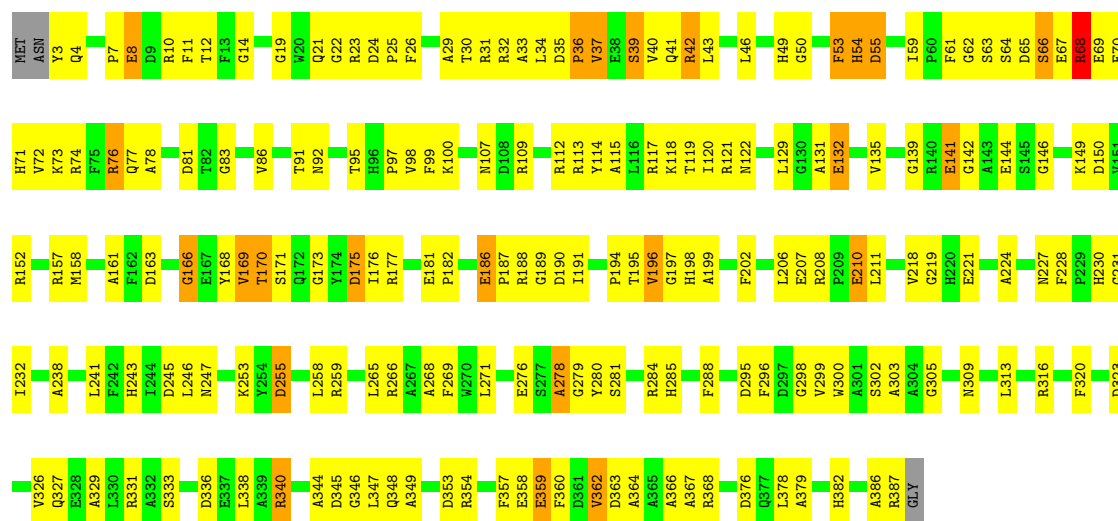
3 Residue-property plots [i](#)

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: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	93.90Å 99.70Å 102.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.00 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (14.00-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3339	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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	1.99	111/3103 (3.6%)	2.19	151/4201 (3.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	5

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	ASP	C-N	-19.91	1.09	1.33
1	A	191	ILE	C-N	19.71	1.59	1.33
1	A	68	ARG	C-N	-14.95	1.14	1.34
1	A	95	THR	C-N	14.87	1.53	1.33
1	A	36	PRO	C-N	14.16	1.51	1.33
1	A	114	TYR	C-N	14.03	1.52	1.33
1	A	298	GLY	C-N	13.95	1.50	1.33
1	A	302	SER	C-N	12.92	1.50	1.33
1	A	280	TYR	C-N	12.79	1.51	1.33
1	A	255	ASP	C-N	12.67	1.52	1.33
1	A	121	ARG	C-N	12.34	1.52	1.33
1	A	320	PHE	C-N	11.65	1.51	1.33
1	A	196	VAL	C-N	11.23	1.47	1.33
1	A	115	ALA	C-N	11.14	1.50	1.33
1	A	30	THR	C-N	10.72	1.48	1.33
1	A	63	SER	C-N	10.60	1.47	1.33
1	A	171	SER	C-N	10.52	1.49	1.33
1	A	135	VAL	C-N	10.51	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	GLY	C-N	-10.34	1.20	1.33
1	A	62	GLY	C-N	10.30	1.47	1.33
1	A	112	ARG	C-N	10.28	1.48	1.33
1	A	92	ASN	C-N	9.98	1.48	1.33
1	A	219	GLY	C-N	9.62	1.47	1.33
1	A	269	PHE	C-N	9.54	1.47	1.33
1	A	278	ALA	C-N	9.52	1.43	1.33
1	A	146	GLY	C-N	9.10	1.48	1.33
1	A	333	SER	C-N	9.05	1.46	1.33
1	A	71	HIS	C-N	-9.04	1.22	1.33
1	A	300	TRP	C-N	8.97	1.45	1.33
1	A	176	ILE	C-N	8.82	1.45	1.33
1	A	119	THR	C-N	8.73	1.45	1.33
1	A	3	TYR	C-N	-8.66	1.15	1.33
1	A	19	GLY	C-N	8.59	1.46	1.33
1	A	224	ALA	C-N	8.49	1.44	1.33
1	A	195	THR	C-N	-8.23	1.24	1.33
1	A	246	LEU	C-N	8.21	1.41	1.33
1	A	367	ALA	C-N	8.11	1.44	1.33
1	A	386	ALA	C-N	-8.01	1.22	1.33
1	A	152	ARG	C-N	7.94	1.44	1.33
1	A	295	ASP	C-N	7.93	1.44	1.34
1	A	25	PRO	C-N	7.85	1.43	1.33
1	A	142	GLY	C-N	7.77	1.43	1.33
1	A	364	ALA	C-N	7.52	1.43	1.33
1	A	241	LEU	C-N	7.49	1.44	1.33
1	A	340	ARG	C-N	7.47	1.43	1.33
1	A	206	LEU	C-N	7.44	1.43	1.33
1	A	129	LEU	C-N	7.40	1.44	1.33
1	A	7	PRO	C-N	7.11	1.43	1.33
1	A	238	ALA	C-N	-7.11	1.24	1.33
1	A	316	ARG	C-N	7.08	1.43	1.33
1	A	113	ARG	C-N	7.03	1.43	1.33
1	A	65	ASP	C-N	7.01	1.44	1.33
1	A	279	GLY	C-N	7.01	1.43	1.33
1	A	54	HIS	C-N	6.99	1.42	1.33
1	A	122	ASN	C-N	6.99	1.42	1.33
1	A	329	ALA	C-N	6.98	1.43	1.33
1	A	187	PRO	C-N	-6.89	1.24	1.33
1	A	46	LEU	C-N	6.86	1.42	1.33
1	A	305	GLY	C-N	6.84	1.42	1.33
1	A	163	ASP	C-N	6.84	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	PHE	C-N	-6.81	1.23	1.33
1	A	378	LEU	C-N	6.77	1.43	1.33
1	A	97	PRO	C-N	6.76	1.41	1.34
1	A	139	GLY	C-N	6.76	1.42	1.33
1	A	353	ASP	C-N	-6.69	1.24	1.33
1	A	230	HIS	C-N	6.63	1.41	1.33
1	A	303	ALA	C-N	6.61	1.42	1.33
1	A	21	GLN	C-N	-6.60	1.25	1.33
1	A	67	GLU	C-N	6.52	1.41	1.33
1	A	299	VAL	C-N	6.51	1.43	1.33
1	A	98	VAL	C-N	6.39	1.41	1.33
1	A	346	GLY	C-N	6.36	1.42	1.33
1	A	207	GLU	C-N	6.31	1.42	1.34
1	A	379	ALA	C-N	6.31	1.41	1.33
1	A	271	LEU	C-N	6.29	1.41	1.33
1	A	309	ASN	C-N	6.29	1.41	1.33
1	A	189	GLY	C-O	6.20	1.31	1.23
1	A	338	LEU	C-N	6.19	1.43	1.33
1	A	99	PHE	C-N	6.17	1.42	1.33
1	A	211	LEU	C-N	6.14	1.43	1.33
1	A	366	ALA	C-N	6.14	1.43	1.33
1	A	42	ARG	C-N	-6.08	1.25	1.33
1	A	83	GLY	C-N	6.04	1.41	1.33
1	A	72	VAL	C-N	6.02	1.41	1.33
1	A	181	GLU	C-N	5.96	1.40	1.33
1	A	358	GLU	C-N	5.91	1.42	1.33
1	A	69	GLU	C-N	-5.90	1.26	1.33
1	A	231	GLY	C-N	-5.89	1.26	1.33
1	A	198	HIS	C-N	-5.85	1.26	1.33
1	A	35	ASP	C-N	5.79	1.47	1.33
1	A	199	ALA	C-O	5.78	1.30	1.24
1	A	55	ASP	C-N	-5.76	1.25	1.33
1	A	326	VAL	C-N	5.72	1.41	1.34
1	A	221	GLU	CA-C	5.51	1.60	1.52
1	A	141	GLU	C-N	5.50	1.40	1.33
1	A	53	PHE	C-N	5.45	1.40	1.33
1	A	118	LYS	C-N	-5.41	1.27	1.33
1	A	158	MET	C-N	-5.38	1.26	1.34
1	A	281	SER	C-N	5.35	1.43	1.33
1	A	288	PHE	C-N	-5.34	1.27	1.33
1	A	363	ASP	C-N	-5.32	1.26	1.33
1	A	197	GLY	C-N	5.29	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	HIS	C-N	5.29	1.38	1.33
1	A	202	PHE	C-N	5.26	1.40	1.34
1	A	173	GLY	C-N	-5.24	1.26	1.33
1	A	73	LYS	C-N	-5.19	1.27	1.33
1	A	120	ILE	C-N	-5.06	1.27	1.33
1	A	107	ASN	C-N	5.05	1.40	1.33
1	A	150	ASP	C-N	5.05	1.40	1.33
1	A	227	ASN	C-N	5.04	1.41	1.33
1	A	144	GLU	C-N	5.04	1.40	1.33

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	GLY	O-C-N	-12.98	106.18	122.41
1	A	168	TYR	O-C-N	-10.73	111.01	122.07
1	A	37	VAL	N-CA-CB	10.46	122.12	110.51
1	A	168	TYR	CA-C-O	10.06	131.38	120.82
1	A	3	TYR	CA-C-N	9.67	145.39	121.80
1	A	3	TYR	C-N-CA	9.67	145.39	121.80
1	A	191	ILE	CA-C-O	9.65	131.72	120.72
1	A	191	ILE	O-C-N	-9.34	113.62	123.14
1	A	367	ALA	CA-C-N	-9.26	107.99	120.95
1	A	367	ALA	C-N-CA	-9.26	107.99	120.95
1	A	76	ARG	NE-CZ-NH2	-9.21	110.91	119.20
1	A	42	ARG	CD-NE-CZ	9.14	137.19	124.40
1	A	10	ARG	CD-NE-CZ	9.08	137.11	124.40
1	A	280	TYR	CA-C-N	-9.00	108.36	122.49
1	A	280	TYR	C-N-CA	-9.00	108.36	122.49
1	A	3	TYR	O-C-N	-8.39	109.57	123.00
1	A	296	PHE	O-C-N	-8.14	112.70	122.22
1	A	327	GLN	OE1-CD-NE2	8.11	130.71	122.60
1	A	265	LEU	CA-C-O	-8.04	110.72	119.97
1	A	37	VAL	N-CA-C	7.99	118.75	110.36
1	A	23	ARG	CD-NE-CZ	7.76	135.26	124.40
1	A	358	GLU	N-CA-C	-7.69	102.90	111.28
1	A	42	ARG	CA-C-N	7.57	131.04	120.29
1	A	42	ARG	C-N-CA	7.57	131.04	120.29
1	A	14	GLY	CA-C-O	-7.55	114.70	121.64
1	A	26	PHE	O-C-N	-7.52	113.30	122.25
1	A	23	ARG	O-C-N	-7.30	114.05	123.02
1	A	39	SER	CA-C-O	-7.27	112.85	120.55
1	A	362	VAL	N-CA-CB	7.25	121.46	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	O-C-N	7.05	131.44	123.27
1	A	41	GLN	CB-CG-CD	6.88	124.29	112.60
1	A	268	ALA	CA-C-N	6.87	129.78	120.44
1	A	268	ALA	C-N-CA	6.87	129.78	120.44
1	A	284	ARG	NE-CZ-NH2	-6.84	113.05	119.20
1	A	266	ARG	NE-CZ-NH1	6.78	128.28	121.50
1	A	367	ALA	O-C-N	6.75	131.99	122.41
1	A	171	SER	CA-C-O	6.73	127.73	119.79
1	A	42	ARG	O-C-N	-6.71	114.50	122.15
1	A	78	ALA	O-C-N	-6.68	114.06	122.27
1	A	78	ALA	CA-C-N	6.67	129.22	120.28
1	A	78	ALA	C-N-CA	6.67	129.22	120.28
1	A	198	HIS	CA-C-O	-6.67	113.76	120.90
1	A	190	ASP	O-C-N	6.64	131.37	123.33
1	A	109	ARG	NE-CZ-NH1	-6.63	114.86	121.50
1	A	333	SER	CA-C-O	6.63	127.31	119.56
1	A	69	GLU	CA-C-N	6.61	129.04	120.44
1	A	69	GLU	C-N-CA	6.61	129.04	120.44
1	A	118	LYS	O-C-N	-6.55	115.18	122.12
1	A	348	GLN	OE1-CD-NE2	6.53	129.13	122.60
1	A	68	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	A	118	LYS	CA-C-N	6.44	129.74	120.79
1	A	118	LYS	C-N-CA	6.44	129.74	120.79
1	A	8	GLU	CA-CB-CG	6.41	126.91	114.10
1	A	194	PRO	O-C-N	-6.37	113.64	122.30
1	A	35	ASP	O-C-N	-6.37	115.63	121.30
1	A	76	ARG	NH1-CZ-NH2	6.35	127.56	119.30
1	A	61	PHE	CA-C-N	6.35	133.54	122.05
1	A	61	PHE	C-N-CA	6.35	133.54	122.05
1	A	331	ARG	NE-CZ-NH2	-6.30	113.53	119.20
1	A	258	LEU	O-C-N	6.29	129.96	122.79
1	A	243	HIS	CA-C-O	-6.23	114.78	121.38
1	A	253	LYS	CA-C-O	-6.22	114.47	120.94
1	A	344	ALA	O-C-N	6.20	130.74	122.43
1	A	121	ARG	CA-C-O	6.18	127.10	120.55
1	A	266	ARG	NE-CZ-NH2	-6.16	113.66	119.20
1	A	266	ARG	CD-NE-CZ	6.05	132.87	124.40
1	A	190	ASP	CA-C-N	-6.01	115.34	123.10
1	A	190	ASP	C-N-CA	-6.01	115.34	123.10
1	A	168	TYR	CA-C-N	6.01	128.69	120.46
1	A	168	TYR	C-N-CA	6.01	128.69	120.46
1	A	329	ALA	CA-C-O	6.01	126.92	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	VAL	O-C-N	-6.00	116.05	121.87
1	A	345	ASP	CA-C-N	5.99	132.38	122.43
1	A	345	ASP	C-N-CA	5.99	132.38	122.43
1	A	378	LEU	CA-C-O	5.86	126.96	120.63
1	A	7	PRO	O-C-N	-5.83	114.38	122.30
1	A	368	ARG	CD-NE-CZ	5.82	132.55	124.40
1	A	100	LYS	CA-C-N	5.81	131.66	122.60
1	A	100	LYS	C-N-CA	5.81	131.66	122.60
1	A	188	ARG	CA-C-N	5.79	126.54	119.99
1	A	188	ARG	C-N-CA	5.79	126.54	119.99
1	A	281	SER	N-CA-C	-5.78	104.89	112.41
1	A	21	GLN	OE1-CD-NE2	5.75	128.35	122.60
1	A	74	ARG	CD-NE-CZ	5.75	132.46	124.40
1	A	173	GLY	CA-C-N	5.74	129.63	121.42
1	A	173	GLY	C-N-CA	5.74	129.63	121.42
1	A	152	ARG	CD-NE-CZ	5.70	132.38	124.40
1	A	349	ALA	O-C-N	5.70	128.65	122.15
1	A	210	GLU	CB-CG-CD	5.70	122.28	112.60
1	A	22	GLY	O-C-N	5.67	128.97	122.33
1	A	296	PHE	CA-C-N	5.63	128.14	120.54
1	A	296	PHE	C-N-CA	5.63	128.14	120.54
1	A	331	ARG	NH1-CZ-NH2	5.62	126.61	119.30
1	A	24	ASP	CA-C-N	5.62	125.29	119.56
1	A	24	ASP	C-N-CA	5.62	125.29	119.56
1	A	66	SER	O-C-N	5.62	129.53	122.23
1	A	14	GLY	O-C-N	5.58	128.66	122.96
1	A	41	GLN	O-C-N	5.58	128.51	122.15
1	A	166	GLY	N-CA-C	-5.56	105.92	113.37
1	A	76	ARG	N-CA-CB	-5.54	101.97	110.12
1	A	316	ARG	O-C-N	-5.52	116.26	122.12
1	A	284	ARG	CA-C-N	-5.48	113.98	122.09
1	A	284	ARG	C-N-CA	-5.48	113.98	122.09
1	A	177	ARG	NE-CZ-NH2	5.47	124.13	119.20
1	A	10	ARG	NH1-CZ-NH2	-5.47	112.19	119.30
1	A	368	ARG	NE-CZ-NH2	-5.47	114.28	119.20
1	A	336	ASP	O-C-N	5.46	127.76	122.09
1	A	188	ARG	O-C-N	-5.44	116.81	122.96
1	A	367	ALA	N-CA-C	-5.44	106.64	113.28
1	A	338	LEU	CA-C-O	5.43	126.24	120.10
1	A	221	GLU	N-CA-C	-5.43	105.52	111.82
1	A	24	ASP	O-C-N	-5.43	115.08	121.32
1	A	359	GLU	CA-C-N	-5.41	113.77	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	GLU	C-N-CA	-5.41	113.77	121.50
1	A	259	ARG	NE-CZ-NH1	5.38	126.88	121.50
1	A	132	GLU	N-CA-CB	-5.37	102.63	110.47
1	A	357	PHE	CA-C-O	5.37	128.18	120.51
1	A	176	ILE	O-C-N	5.33	129.27	123.09
1	A	122	ASN	CA-CB-CG	-5.31	107.29	112.60
1	A	117	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	A	176	ILE	CA-C-O	-5.29	115.24	120.90
1	A	11	PHE	CA-CB-CG	5.29	119.08	113.80
1	A	64	SER	O-C-N	5.28	129.09	122.65
1	A	247	ASN	N-CA-CB	5.28	118.00	110.51
1	A	92	ASN	CA-C-O	5.27	126.67	120.98
1	A	269	PHE	N-CA-C	-5.25	105.47	111.14
1	A	243	HIS	CA-CB-CG	5.23	119.03	113.80
1	A	81	ASP	N-CA-C	-5.21	106.42	112.89
1	A	8	GLU	O-C-N	-5.21	115.45	122.43
1	A	41	GLN	CA-C-N	-5.20	112.90	120.29
1	A	41	GLN	C-N-CA	-5.20	112.90	120.29
1	A	29	ALA	O-C-N	-5.19	116.64	122.97
1	A	77	GLN	CA-C-N	-5.17	112.45	120.31
1	A	77	GLN	C-N-CA	-5.17	112.45	120.31
1	A	182	PRO	CA-C-O	-5.13	115.60	121.86
1	A	161	ALA	N-CA-C	-5.13	105.60	111.14
1	A	224	ALA	N-CA-C	-5.13	106.71	113.17
1	A	68	ARG	CG-CD-NE	5.13	123.28	112.00
1	A	376	ASP	CA-C-O	5.12	125.98	120.55
1	A	157	ARG	CA-C-O	5.08	125.94	120.55
1	A	12	THR	CA-C-O	-5.07	115.51	121.44
1	A	149	LYS	CA-C-N	-5.07	115.45	122.30
1	A	149	LYS	C-N-CA	-5.07	115.45	122.30
1	A	382	HIS	N-CA-C	5.05	116.48	111.07
1	A	95	THR	CA-C-O	5.03	126.08	120.90
1	A	195	THR	CA-C-N	5.03	127.36	120.77
1	A	195	THR	C-N-CA	5.03	127.36	120.77
1	A	300	TRP	CA-C-O	5.02	125.56	119.38
1	A	265	LEU	CB-CA-C	-5.01	101.05	110.67
1	A	276	GLU	CA-C-N	-5.01	112.38	121.14
1	A	276	GLU	C-N-CA	-5.01	112.38	121.14

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
1	A	37	VAL	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	THR	Mainchain
1	A	196	VAL	Mainchain
1	A	210	GLU	Mainchain
1	A	278	ALA	Mainchain
1	A	53	PHE	Peptide

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	3031	0	2897	18	0
2	A	10	0	9	0	0
3	A	2	0	0	0	0
4	A	296	0	0	4	0
All	All	3339	0	2906	18	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 3.

All (18) 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:59:ILE:HG21	1:A:68:ARG:HG2	1.73	0.71
1:A:354:ARG:HB3	1:A:359:GLU:HG3	1.79	0.64
1:A:340:ARG:HD2	4:A:637:HOH:O	1.98	0.63
1:A:141:GLU:OE2	4:A:587:HOH:O	2.17	0.58
1:A:186:GLU:OE1	1:A:255:ASP:HB3	2.08	0.54
1:A:166:GLY:O	1:A:170:THR:HG23	2.08	0.52
1:A:32:ARG:NH1	1:A:33:ALA:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ARG:CD	4:A:637:HOH:O	2.58	0.48
1:A:36:PRO:O	1:A:40:VAL:HG23	2.14	0.47
1:A:245:ASP:OD1	1:A:285:HIS:HD2	1.98	0.47
1:A:86:VAL:O	1:A:131:ALA:HA	2.17	0.45
1:A:228:PHE:CZ	1:A:232:ILE:HD11	2.52	0.44
1:A:360:PHE:CD2	1:A:362:VAL:HG12	2.53	0.44
1:A:208:ARG:NH1	4:A:582:HOH:O	2.34	0.43
1:A:323:ASP:OD2	1:A:387:ARG:NH2	2.47	0.43
1:A:354:ARG:NE	1:A:359:GLU:OE2	2.52	0.41
1:A:54:HIS:O	1:A:55:ASP:C	2.63	0.41
1:A:34:LEU:HD13	1:A:39:SER:OG	2.21	0.41

There are no symmetry-related clashes.

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	383/388 (99%)	369 (96%)	12 (3%)	2 (0%)	24	12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLU
1	A	218	VAL

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	302/304 (99%)	287 (95%)	15 (5%)	22 8

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	8	GLU
1	A	37	VAL
1	A	42	ARG
1	A	43	LEU
1	A	66	SER
1	A	68	ARG
1	A	70	GLU
1	A	76	ARG
1	A	91	THR
1	A	132	GLU
1	A	169	VAL
1	A	175	ASP
1	A	313	LEU
1	A	347	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	71	HIS
1	A	285	HIS
1	A	348	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	389	3	9,9,9	1.44	2 (22%)	11,11,11	1.51	2 (18%)

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	389	3	-	0/12/12/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	389	XYL	O1-C1	-3.26	1.28	1.42
2	A	389	XYL	O2-C2	-2.70	1.37	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	389	XYL	O5-C5-C4	2.78	116.99	111.16
2	A	389	XYL	O1-C1-C2	-2.27	106.38	111.16

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3:TYR	C	4:GLN	N	1.15
1	A	68:ARG	C	69:GLU	N	1.13
1	A	175:ASP	C	176:ILE	N	1.09

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.