



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:56 PM UTC

PDB ID : 1XIJ / pdb_00001xij
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

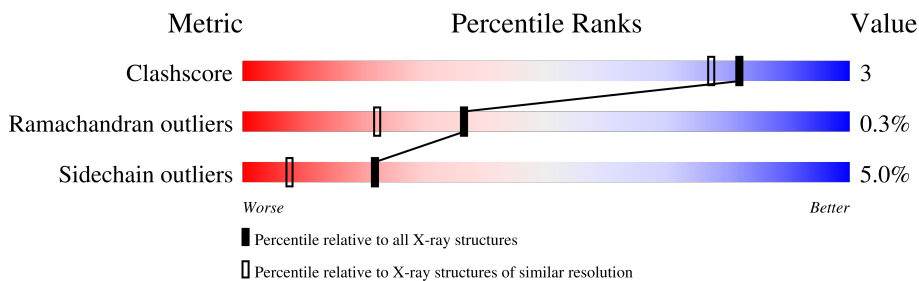
1 Overall quality at a glance

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	THE	A	389	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3418 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.

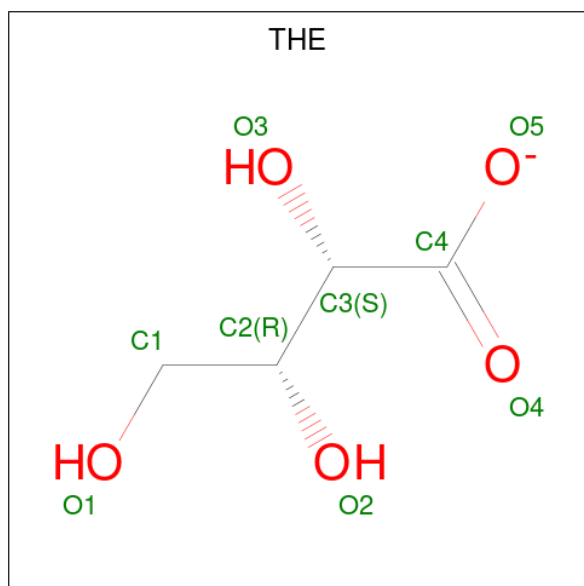
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

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

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 THREONATE ION (CCD ID: THE) (formula: $C_4H_7O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mn 1	0	0

- Molecule 4 is water.

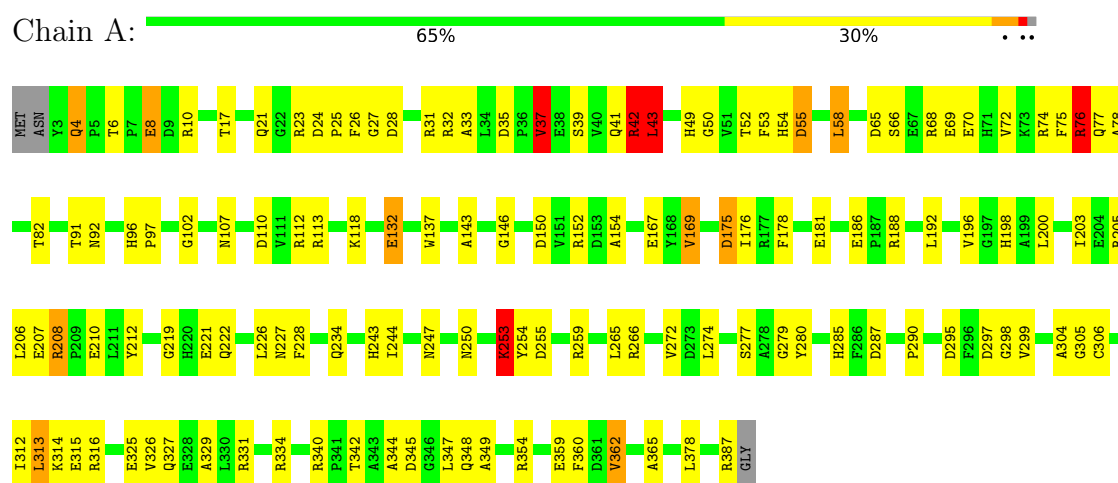
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	377	Total 377	O 377	0	0

3 Residue-property plots

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



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	93.88Å 99.68Å 102.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.156 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3418	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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: THE, 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	1.51	22/3103 (0.7%)	2.27	144/4201 (3.4%)

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	0	1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	GLY	C-O	8.11	1.30	1.23
1	A	50	GLY	C-N	-7.03	1.24	1.33
1	A	17	THR	C-O	6.59	1.29	1.23
1	A	227	ASN	N-CA	6.07	1.53	1.46
1	A	28	ASP	C-N	5.99	1.41	1.33
1	A	326	VAL	C-O	5.84	1.30	1.24
1	A	37	VAL	N-CA	5.79	1.53	1.46
1	A	198	HIS	CE1-NE2	5.65	1.38	1.32
1	A	255	ASP	N-CA	5.58	1.53	1.46
1	A	340	ARG	CD-NE	-5.55	1.38	1.46
1	A	304	ALA	C-O	5.43	1.30	1.24
1	A	221	GLU	CD-OE2	-5.29	1.15	1.25
1	A	219	GLY	CA-C	5.26	1.58	1.51
1	A	234	GLN	C-O	5.25	1.30	1.24
1	A	42	ARG	N-CA	5.24	1.52	1.46
1	A	222	GLN	C-O	5.22	1.30	1.24
1	A	259	ARG	CD-NE	5.19	1.53	1.46
1	A	200	LEU	N-CA	5.17	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	GLY	C-O	5.17	1.29	1.24
1	A	253	LYS	CA-C	-5.16	1.46	1.53
1	A	192	LEU	C-O	5.10	1.30	1.23
1	A	285	HIS	ND1-CE1	5.08	1.37	1.32

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ARG	CD-NE-CZ	25.48	160.08	124.40
1	A	387	ARG	CA-C-O	17.92	151.27	120.80
1	A	340	ARG	NE-CZ-NH1	16.56	138.06	121.50
1	A	10	ARG	CD-NE-CZ	15.57	146.19	124.40
1	A	340	ARG	NE-CZ-NH2	-13.12	107.40	119.20
1	A	76	ARG	NE-CZ-NH2	-12.18	108.24	119.20
1	A	387	ARG	CD-NE-CZ	11.68	140.75	124.40
1	A	143	ALA	O-C-N	10.50	134.65	123.42
1	A	76	ARG	NH1-CZ-NH2	10.46	132.90	119.30
1	A	68	ARG	NE-CZ-NH2	10.07	128.27	119.20
1	A	265	LEU	CA-C-O	-9.69	110.28	120.55
1	A	42	ARG	CD-NE-CZ	9.22	137.31	124.40
1	A	23	ARG	CD-NE-CZ	8.38	136.13	124.40
1	A	331	ARG	NH1-CZ-NH2	8.17	129.92	119.30
1	A	342	THR	O-C-N	7.87	131.13	122.15
1	A	210	GLU	CB-CG-CD	7.83	125.91	112.60
1	A	331	ARG	NE-CZ-NH2	-7.78	112.20	119.20
1	A	21	GLN	OE1-CD-NE2	7.76	130.37	122.60
1	A	348	GLN	OE1-CD-NE2	7.65	130.25	122.60
1	A	146	GLY	O-C-N	-7.59	114.82	122.19
1	A	92	ASN	CA-CB-CG	-7.58	105.02	112.60
1	A	4	GLN	CB-CG-CD	7.56	125.45	112.60
1	A	143	ALA	CA-C-O	-7.44	113.27	121.23
1	A	4	GLN	OE1-CD-NE2	-7.31	115.29	122.60
1	A	345	ASP	CA-CB-CG	7.30	119.90	112.60
1	A	314	LYS	O-C-N	7.15	129.44	122.07
1	A	287	ASP	CA-CB-CG	-7.12	105.48	112.60
1	A	76	ARG	CG-CD-NE	-7.11	96.36	112.00
1	A	132	GLU	N-CA-CB	-7.08	100.12	110.53
1	A	175	ASP	CA-CB-CG	-7.03	105.57	112.60
1	A	266	ARG	NE-CZ-NH2	-7.00	112.90	119.20
1	A	24	ASP	CA-CB-CG	6.93	119.53	112.60
1	A	297	ASP	CA-CB-CG	-6.93	105.67	112.60
1	A	298	GLY	CA-C-O	-6.87	112.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	PHE	O-C-N	6.86	126.59	120.48
1	A	243	HIS	CA-C-O	-6.86	114.11	121.38
1	A	272	VAL	O-C-N	6.80	128.46	121.87
1	A	6	THR	O-C-N	6.79	127.13	121.35
1	A	299	VAL	O-C-N	6.79	128.56	121.91
1	A	169	VAL	N-CA-CB	-6.78	101.31	110.54
1	A	176	ILE	O-C-N	6.75	130.92	123.09
1	A	4	GLN	CA-C-O	6.73	126.86	119.32
1	A	176	ILE	N-CA-C	-6.72	99.48	108.35
1	A	315	GLU	CA-C-N	6.66	129.20	120.28
1	A	315	GLU	C-N-CA	6.66	129.20	120.28
1	A	24	ASP	CB-CA-C	6.64	123.24	110.17
1	A	203	ILE	O-C-N	6.57	128.50	121.87
1	A	8	GLU	CA-CB-CG	6.55	127.20	114.10
1	A	378	LEU	O-C-N	-6.49	115.24	122.12
1	A	154	ALA	CA-C-O	-6.49	113.67	120.55
1	A	74	ARG	NE-CZ-NH2	-6.47	113.38	119.20
1	A	152	ARG	NE-CZ-NH2	-6.46	113.39	119.20
1	A	82	THR	O-C-N	6.44	130.28	122.48
1	A	226	LEU	CA-C-O	-6.44	114.12	121.72
1	A	228	PHE	CA-C-O	-6.29	112.56	118.73
1	A	362	VAL	CA-C-O	-6.26	113.49	120.25
1	A	50	GLY	CA-C-O	-6.25	115.54	121.60
1	A	28	ASP	O-C-N	6.19	130.26	122.65
1	A	365	ALA	CA-C-O	-6.17	114.34	120.82
1	A	327	GLN	OE1-CD-NE2	6.16	128.76	122.60
1	A	365	ALA	O-C-N	6.15	128.41	122.07
1	A	277	SER	CB-CA-C	6.13	122.88	110.38
1	A	107	ASN	OD1-CG-ND2	-6.04	116.56	122.60
1	A	55	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	52	THR	CA-C-O	-6.03	114.58	121.58
1	A	192	LEU	CA-C-O	-6.03	114.98	121.56
1	A	110	ASP	CA-CB-CG	5.98	118.58	112.60
1	A	178	PHE	CA-CB-CG	-5.97	107.83	113.80
1	A	315	GLU	O-C-N	-5.96	115.93	122.07
1	A	112	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	A	68	ARG	NH1-CZ-NH2	-5.94	111.58	119.30
1	A	207	GLU	CA-C-O	-5.93	114.26	120.55
1	A	35	ASP	CA-C-O	-5.92	113.88	119.80
1	A	74	ARG	CD-NE-CZ	5.89	132.64	124.40
1	A	326	VAL	O-C-N	-5.88	115.78	121.90
1	A	17	THR	CA-C-O	-5.86	114.26	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ASP	CB-CA-C	5.84	121.44	110.63
1	A	49	HIS	N-CA-CB	-5.82	101.97	110.47
1	A	349	ALA	O-C-N	5.79	128.26	122.12
1	A	137	TRP	CA-C-O	-5.79	114.59	120.84
1	A	331	ARG	CG-CD-NE	-5.78	99.30	112.00
1	A	305	GLY	CA-C-O	-5.76	114.18	120.40
1	A	340	ARG	CA-C-O	-5.76	115.36	120.19
1	A	219	GLY	CA-C-O	-5.68	114.05	120.30
1	A	334	ARG	NE-CZ-NH2	-5.68	114.09	119.20
1	A	274	LEU	N-CA-C	5.67	117.13	111.07
1	A	280	TYR	CA-C-N	-5.66	113.65	122.37
1	A	280	TYR	C-N-CA	-5.66	113.65	122.37
1	A	207	GLU	CA-CB-CG	-5.65	102.81	114.10
1	A	290	PRO	CB-CA-C	5.65	117.81	110.92
1	A	4	GLN	CG-CD-NE2	5.64	124.86	116.40
1	A	327	GLN	CA-C-O	-5.63	114.55	120.63
1	A	10	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	A	250	ASN	CA-CB-CG	-5.61	106.99	112.60
1	A	196	VAL	CA-C-O	-5.60	115.44	121.27
1	A	316	ARG	CA-C-O	-5.56	114.66	120.55
1	A	150	ASP	CA-C-O	-5.55	114.33	120.60
1	A	208	ARG	CB-CG-CD	-5.53	98.58	111.30
1	A	312	ILE	CA-C-O	-5.49	115.35	121.17
1	A	10	ARG	NH1-CZ-NH2	-5.49	112.17	119.30
1	A	344	ALA	O-C-N	5.48	129.77	122.43
1	A	266	ARG	CD-NE-CZ	5.42	132.00	124.40
1	A	188	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	A	208	ARG	CA-C-N	5.39	125.05	119.56
1	A	208	ARG	C-N-CA	5.39	125.05	119.56
1	A	152	ARG	CA-CB-CG	-5.38	103.33	114.10
1	A	244	ILE	CA-C-O	-5.35	115.68	121.19
1	A	50	GLY	N-CA-C	5.34	119.31	110.55
1	A	132	GLU	CA-CB-CG	5.34	124.78	114.10
1	A	41	GLN	CB-CG-CD	5.33	121.66	112.60
1	A	37	VAL	CA-C-O	-5.31	114.74	120.47
1	A	342	THR	CA-C-N	-5.31	110.32	122.95
1	A	342	THR	C-N-CA	-5.31	110.32	122.95
1	A	176	ILE	CA-C-O	-5.27	115.26	120.90
1	A	378	LEU	CA-C-O	5.27	126.13	120.55
1	A	77	GLN	CA-C-O	-5.26	114.97	120.55
1	A	313	LEU	N-CA-CB	-5.26	102.12	110.28
1	A	206	LEU	CA-C-O	-5.25	115.61	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	GLY	O-C-N	-5.25	117.79	122.57
1	A	295	ASP	OD1-CG-OD2	-5.25	110.31	122.90
1	A	181	GLU	O-C-N	5.24	127.79	121.29
1	A	72	VAL	CA-C-O	-5.24	115.23	121.05
1	A	113	ARG	CD-NE-CZ	5.24	131.73	124.40
1	A	43	LEU	N-CA-CB	-5.21	102.45	110.16
1	A	254	TYR	CA-C-O	-5.21	115.81	121.44
1	A	349	ALA	CB-CA-C	-5.21	102.14	110.79
1	A	312	ILE	O-C-N	5.20	127.00	121.91
1	A	250	ASN	CA-C-O	-5.18	116.42	122.37
1	A	31	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	A	247	ASN	CA-C-N	5.16	125.58	121.61
1	A	247	ASN	C-N-CA	5.16	125.58	121.61
1	A	325	GLU	O-C-N	5.16	128.03	122.15
1	A	306	CYS	O-C-N	5.16	127.45	122.09
1	A	329	ALA	O-C-N	-5.13	116.68	122.12
1	A	69	GLU	CA-C-N	5.12	127.55	120.29
1	A	69	GLU	C-N-CA	5.12	127.55	120.29
1	A	247	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	76	ARG	CB-CG-CD	-5.09	99.60	111.30
1	A	58	LEU	N-CA-C	-5.07	106.78	113.12
1	A	167	GLU	CB-CA-C	5.06	119.19	110.79
1	A	198	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	A	27	GLY	O-C-N	5.01	127.08	123.27
1	A	118	LYS	CA-C-N	5.00	126.94	120.44
1	A	118	LYS	C-N-CA	5.00	126.94	120.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	2900	15	2
2	A	9	0	6	0	0
3	A	1	0	0	0	0
4	A	377	0	0	4	4
All	All	3418	0	2906	15	4

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 (15) 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:25:PRO:HG2	1:A:26:PHE:CD1	2.39	0.57
1:A:25:PRO:HG2	1:A:26:PHE:CE1	2.48	0.47
1:A:32:ARG:NH1	1:A:33:ALA:O	2.47	0.47
1:A:54:HIS:O	1:A:55:ASP:C	2.58	0.46
1:A:42:ARG:HE	1:A:42:ARG:HA	1.82	0.45
1:A:37:VAL:HB	1:A:78:ALA:HB2	1.98	0.45
1:A:205:ARG:HD2	4:A:772:HOH:O	2.16	0.45
1:A:58:LEU:HD11	1:A:75:PHE:CG	2.52	0.45
1:A:212:TYR:HB3	4:A:739:HOH:O	2.18	0.44
1:A:76:ARG:HD3	4:A:770:HOH:O	2.17	0.44
1:A:208:ARG:NH1	4:A:582:HOH:O	2.35	0.42
1:A:360:PHE:CD2	1:A:362:VAL:HG12	2.55	0.42
1:A:39:SER:O	1:A:43:LEU:HB2	2.21	0.41
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.36	0.41
1:A:354:ARG:HB3	1:A:359:GLU:HG3	2.03	0.40

All (4) 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:A:253:LYS:NZ	4:A:737:HOH:O[4_566]	1.97	0.23
4:A:509:HOH:O	4:A:733:HOH:O[6_555]	2.05	0.15
4:A:629:HOH:O	4:A:715:HOH:O[3_656]	2.11	0.09
1:A:253:LYS:CE	4:A:737:HOH:O[4_566]	2.12	0.08

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%)	372 (97%)	10 (3%)	1 (0%)	36	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	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	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	70	GLU
1	A	76	ARG
1	A	91	THR
1	A	132	GLU

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Mol	Chain	Res	Type
1	A	169	VAL
1	A	175	ASP
1	A	253	LYS
1	A	313	LEU
1	A	347	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	234	GLN
1	A	348	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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	THE	A	389	3	8,8,8	2.83	5 (62%)	8,10,10	4.57	6 (75%)

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	THE	A	389	3	-	5/10/10/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	389	THE	C2-C3	5.91	1.60	1.53
2	A	389	THE	O2-C2	3.09	1.49	1.43
2	A	389	THE	O5-C4	-2.52	1.22	1.30
2	A	389	THE	O3-C3	2.28	1.46	1.42
2	A	389	THE	C3-C4	-2.16	1.49	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	389	THE	O5-C4-O4	-9.28	103.02	124.08
2	A	389	THE	O5-C4-C3	7.12	133.10	113.31
2	A	389	THE	O2-C2-C1	-3.73	100.54	109.03
2	A	389	THE	O3-C3-C4	2.47	115.98	110.69
2	A	389	THE	O3-C3-C2	2.34	115.44	109.46
2	A	389	THE	O1-C1-C2	-2.03	106.89	111.16

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	389	THE	O2-C2-C3-C4
2	A	389	THE	O3-C3-C4-O5
2	A	389	THE	O3-C3-C4-O4
2	A	389	THE	C2-C3-C4-O5
2	A	389	THE	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

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.