



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:11 am BST

PDB ID : 2GYI  
Title : DESIGN, SYNTHESIS, AND CHARACTERIZATION OF A POTENT  
XYLOSE ISOMERASE INHIBITOR, D-THREONOHYDROXAMIC ACID,  
AND HIGH-RESOLUTION X-RAY CRYSTALLOGRAPHIC STRUCTURE  
OF THE ENZYME-INHIBITOR COMPLEX  
Authors : Allen, K.N.; Lavie, A.; Petsko, G.A.; Ringe, D.  
Deposited on : 1994-09-01  
Resolution : 1.60 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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) : 2.11

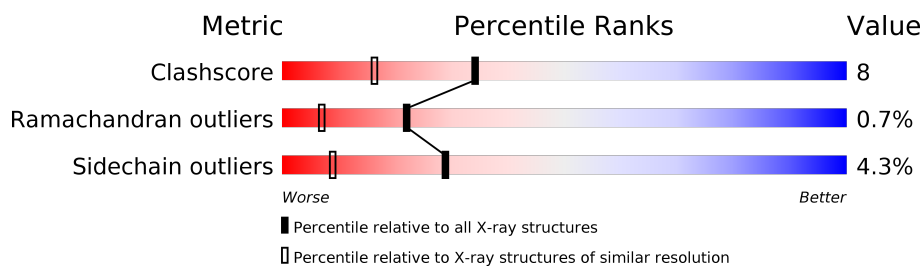
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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  $\geq 3$ , 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	386	
1	B	386	

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
3	HYA	A	960	X	-	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6694 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.

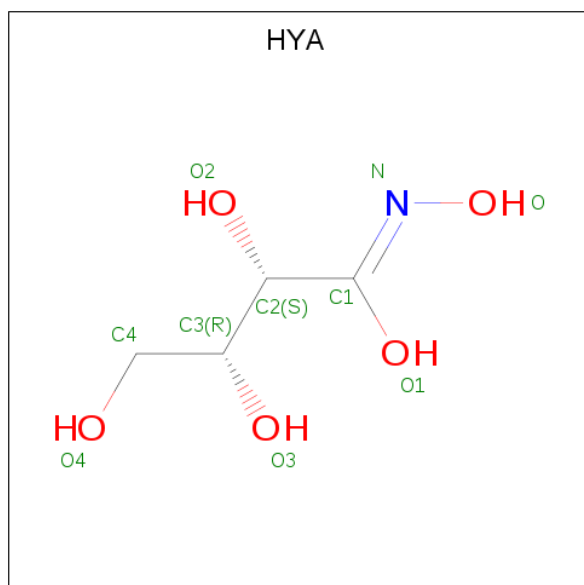
- Molecule 1 is a protein called XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			3018	1901	539	570	8			
1	B	385	Total	C	N	O	S	0	0	0
			3018	1901	539	570	8			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 2,3,4,N-TETRAHYDROXY-BUTYRIMIDIC ACID (three-letter code: HYA) (formula: C<sub>4</sub>H<sub>9</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	4	1	5		
3	B	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 4 is water.

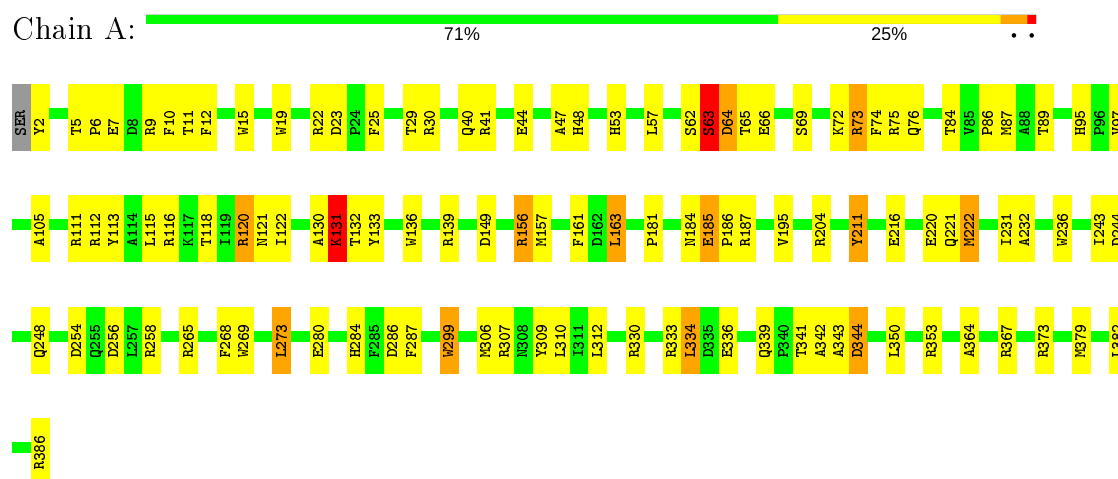
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	303	Total	O	0	0
			303	303		
4	B	331	Total	O	0	0
			331	331		

### 3 Residue-property plots

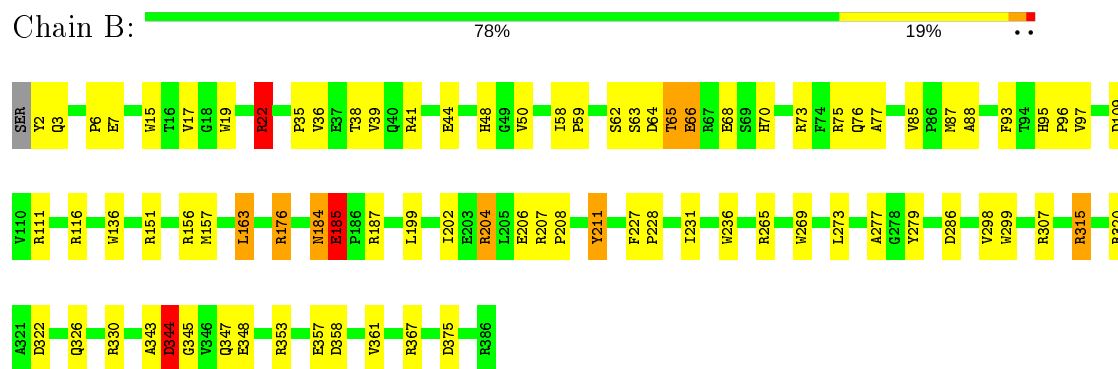
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: XYLOSE ISOMERASE



#### • Molecule 1: XYLOSE ISOMERASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.90 Å 99.05 Å 93.65 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.216 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6694	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	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: HYA, MG

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	1.06	6/3090 (0.2%)	1.61	63/4189 (1.5%)
1	B	0.93	2/3090 (0.1%)	1.57	52/4189 (1.2%)
All	All	1.00	8/6180 (0.1%)	1.59	115/8378 (1.4%)

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	3
1	B	0	2
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	ASP	C-N	24.36	1.90	1.34
1	A	63	SER	C-N	-19.08	0.90	1.34
1	B	66	GLU	CG-CD	11.42	1.69	1.51
1	B	66	GLU	CB-CG	9.44	1.70	1.52
1	A	149	ASP	C-N	-9.28	1.12	1.34
1	A	131	LYS	C-N	7.68	1.51	1.34
1	A	216	GLU	CD-OE1	-5.98	1.19	1.25
1	A	130	ALA	C-N	5.16	1.46	1.34

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ASP	O-C-N	-23.17	85.63	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	ARG	NE-CZ-NH2	-19.68	110.46	120.30
1	B	265	ARG	NE-CZ-NH1	16.80	128.70	120.30
1	A	63	SER	C-N-CA	15.95	161.57	121.70
1	A	112	ARG	NE-CZ-NH1	11.21	125.91	120.30
1	A	63	SER	O-C-N	-10.53	105.85	122.70
1	B	176	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	B	116	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	A	330	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	A	265	ARG	NE-CZ-NH2	-8.65	115.98	120.30
1	B	151	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	B	204	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	131	LYS	O-C-N	-8.31	109.40	122.70
1	A	269	TRP	CD1-CG-CD2	8.18	112.84	106.30
1	A	15	TRP	CD1-CG-CD2	7.91	112.63	106.30
1	A	299	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	A	367	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	A	15	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	B	269	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	A	204	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	B	111	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	B	15	TRP	CE2-CD2-CG	-7.34	101.42	107.30
1	A	236	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	A	299	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	367	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	136	TRP	CD1-CG-CD2	7.22	112.08	106.30
1	A	334	LEU	CA-CB-CG	-7.19	98.75	115.30
1	B	269	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	B	116	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	B	15	TRP	CD1-CG-CD2	6.97	111.88	106.30
1	A	236	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	A	265	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	344	ASP	N-CA-CB	6.83	122.90	110.60
1	A	269	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	A	222	MET	CA-CB-CG	-6.82	101.71	113.30
1	A	15	TRP	CG-CD2-CE3	6.82	140.03	133.90
1	A	136	TRP	CE2-CD2-CG	-6.77	101.88	107.30
1	B	320	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	344	ASP	CA-CB-CG	6.69	128.12	113.40
1	A	75	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	A	19	TRP	CD1-CG-CD2	6.48	111.48	106.30
1	B	299	TRP	CD1-CG-CD2	6.48	111.48	106.30
1	B	330	ARG	NE-CZ-NH1	6.48	123.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	136	TRP	CD1-CG-CD2	6.32	111.36	106.30
1	B	236	TRP	CD1-CG-CD2	6.32	111.36	106.30
1	A	9	ARG	CA-CB-CG	6.31	127.28	113.40
1	A	211	TYR	CB-CG-CD1	-6.30	117.22	121.00
1	B	73	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	22	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	73	ARG	NE-CZ-NH2	6.27	123.44	120.30
1	A	299	TRP	CB-CG-CD1	-6.21	118.92	127.00
1	A	353	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	386	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	15	TRP	CB-CG-CD1	-6.15	119.00	127.00
1	A	379	MET	CG-SD-CE	-6.14	90.38	100.20
1	A	41	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	163	LEU	CA-CB-CG	6.10	129.33	115.30
1	B	156	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	19	TRP	CE2-CD2-CG	-6.09	102.43	107.30
1	A	269	TRP	CG-CD1-NE1	-6.05	104.05	110.10
1	A	269	TRP	CB-CG-CD1	-6.05	119.14	127.00
1	B	279	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	B	286	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	299	TRP	CE2-CD2-CG	-6.00	102.50	107.30
1	B	236	TRP	CE2-CD2-CG	-5.98	102.52	107.30
1	A	30	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	386	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	B	344	ASP	CB-CA-C	-5.94	98.52	110.40
1	A	19	TRP	CE2-CD2-CG	-5.93	102.56	107.30
1	B	273	LEU	CA-CB-CG	5.90	128.88	115.30
1	A	63	SER	CA-C-N	5.90	130.19	117.20
1	B	345	GLY	CA-C-N	-5.88	104.25	117.20
1	B	176	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	B	19	TRP	CD1-CG-CD2	5.81	110.95	106.30
1	B	187	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	343	ALA	N-CA-C	-5.77	95.43	111.00
1	A	120	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	65	THR	O-C-N	5.71	131.84	122.70
1	A	299	TRP	CG-CD2-CE3	5.70	139.03	133.90
1	B	76	GLN	CB-CA-C	-5.70	99.01	110.40
1	B	207	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	187	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	136	TRP	CE2-CD2-CG	-5.66	102.77	107.30
1	A	244	ASP	CB-CG-OD1	5.64	123.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	111	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	269	TRP	CG-CD2-CE3	5.61	138.95	133.90
1	B	75	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	109	ASP	CA-CB-CG	5.60	125.73	113.40
1	A	113	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	A	136	TRP	CG-CD2-CE3	5.59	138.93	133.90
1	B	269	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	A	258	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	353	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	307	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	315	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	B	298	VAL	CA-CB-CG2	-5.36	102.86	110.90
1	B	279	TYR	CB-CG-CD1	5.32	124.19	121.00
1	B	211	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	B	343	ALA	N-CA-C	-5.28	96.75	111.00
1	B	307	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	309	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	A	136	TRP	CG-CD1-NE1	-5.23	104.87	110.10
1	B	299	TRP	CG-CD1-NE1	-5.18	104.92	110.10
1	B	76	GLN	CA-CB-CG	5.15	124.74	113.40
1	B	157	MET	CG-SD-CE	-5.15	91.96	100.20
1	B	322	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	299	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	A	156	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	130	ALA	O-C-N	-5.06	114.60	122.70
1	B	375	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	157	MET	CG-SD-CE	-5.03	92.14	100.20
1	A	2	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	A	204	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	LYS	Mainchain
1	A	364	ALA	Mainchain
1	A	63	SER	Peptide
1	B	22	ARG	Sidechain
1	B	63	SER	Mainchain

## 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	3018	0	2898	65	0
1	B	3018	0	2901	38	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	10	0	8	1	0
3	B	10	0	8	0	0
4	A	303	0	0	16	0
4	B	331	0	0	20	0
All	All	6694	0	5815	100	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 8.

All (100) 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:5:THR:HG23	1:A:7:GLU:CG	1.61	1.29
1:A:64:ASP:C	1:A:65:THR:N	1.90	1.25
1:A:69:SER:OG	1:A:73:ARG:NH2	1.81	1.13
1:A:5:THR:CG2	1:A:7:GLU:CG	2.28	1.11
1:A:5:THR:HG23	1:A:7:GLU:HG2	1.32	1.10
1:A:5:THR:HG23	1:A:7:GLU:HG3	1.33	1.04
1:B:176:ARG:NH1	4:B:1624:HOH:O	1.88	0.97
1:B:48:HIS:ND1	4:B:1622:HOH:O	2.00	0.94
1:A:5:THR:HG21	1:A:7:GLU:OE2	1.71	0.90
1:A:5:THR:CG2	1:A:7:GLU:HG3	1.97	0.86
1:A:5:THR:HG21	1:A:7:GLU:CD	1.95	0.85
1:A:69:SER:CB	1:A:73:ARG:NH2	2.40	0.83
1:B:70:HIS:HD2	4:B:1415:HOH:O	1.62	0.82
1:A:5:THR:CG2	1:A:7:GLU:HG2	2.04	0.79
1:A:5:THR:OG1	1:A:6:PRO:CD	2.34	0.75
1:A:64:ASP:O	1:A:65:THR:N	2.19	0.73
1:A:5:THR:CG2	1:A:7:GLU:CD	2.56	0.73
1:A:341:THR:HG22	4:A:1598:HOH:O	1.89	0.72
1:A:95:HIS:HD2	1:A:97:VAL:H	1.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:GLN:HB2	4:A:1601:HOH:O	1.92	0.69
1:A:299:TRP:O	4:A:1586:HOH:O	2.09	0.69
1:A:5:THR:OG1	1:A:6:PRO:HD2	1.93	0.69
1:A:48:HIS:HB2	4:A:1596:HOH:O	1.93	0.69
1:B:358:ASP:OD1	4:B:1432:HOH:O	2.12	0.67
1:B:163:LEU:HD13	4:B:1412:HOH:O	1.95	0.66
1:B:95:HIS:HD2	1:B:97:VAL:H	1.43	0.65
1:A:306:MET:SD	4:A:1488:HOH:O	2.55	0.64
1:A:69:SER:HB2	1:A:73:ARG:NH2	2.12	0.63
1:B:64:ASP:O	1:B:68:GLU:HG2	1.98	0.63
1:A:73:ARG:HD2	4:A:1499:HOH:O	1.99	0.62
1:B:344:ASP:HB2	4:B:1414:HOH:O	1.99	0.62
1:A:69:SER:O	1:A:72:LYS:HG2	2.00	0.61
1:B:35:PRO:O	1:B:39:VAL:HG23	2.02	0.60
1:A:47:ALA:HA	1:A:306:MET:HE1	1.83	0.60
1:A:63:SER:HB2	4:A:1633:HOH:O	2.02	0.60
1:B:348:GLU:HG3	4:B:1632:HOH:O	2.01	0.59
1:B:36:VAL:HG13	1:B:77:ALA:HB2	1.85	0.58
1:B:50:VAL:HG23	1:B:85:VAL:HG22	1.84	0.58
1:A:84:THR:O	4:A:1620:HOH:O	2.17	0.58
1:B:62:SER:O	4:B:1428:HOH:O	2.17	0.57
1:B:36:VAL:HG23	4:B:1543:HOH:O	2.04	0.55
1:A:342:ALA:HB2	4:A:1598:HOH:O	2.06	0.55
1:B:208:PRO:HG2	4:B:1546:HOH:O	2.05	0.55
1:A:232:ALA:HB2	1:A:273:LEU:HD11	1.90	0.53
1:B:48:HIS:CG	4:B:1622:HOH:O	2.53	0.53
1:B:22:ARG:HD3	4:B:1532:HOH:O	2.08	0.53
1:B:353:ARG:NH2	4:B:1609:HOH:O	2.42	0.52
1:A:195:VAL:HG23	1:A:220:GLU:CD	2.31	0.51
1:B:227:PHE:HB3	1:B:228:PRO:HD3	1.91	0.51
1:B:326:GLN:HG2	4:B:1451:HOH:O	2.11	0.51
1:A:333:ARG:HB3	1:A:336:GLU:HB2	1.92	0.51
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.93	0.51
1:B:70:HIS:CD2	4:B:1415:HOH:O	2.49	0.49
1:A:29:THR:HG22	1:B:96:PRO:HB3	1.95	0.49
1:A:118:THR:O	1:A:122:ILE:HG13	2.13	0.49
1:A:222:MET:SD	1:A:254:ASP:HB3	2.52	0.49
1:B:277:ALA:HB3	4:B:1558:HOH:O	2.13	0.49
1:B:367:ARG:HD2	4:B:1571:HOH:O	2.13	0.48
1:A:268:PHE:HA	1:A:312:LEU:HD22	1.95	0.48
1:A:243:ILE:O	1:A:284:HIS:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ARG:HH11	1:B:367:ARG:HG2	1.79	0.47
1:A:22:ARG:HG3	4:A:1478:HOH:O	2.15	0.47
1:A:47:ALA:HB1	4:A:1593:HOH:O	2.14	0.47
1:A:121:ASN:HB3	1:A:133:TYR:OH	2.16	0.46
1:A:105:ALA:O	1:A:111:ARG:HD3	2.15	0.46
1:B:77:ALA:HA	4:B:1418:HOH:O	2.15	0.45
1:A:95:HIS:CD2	1:A:97:VAL:H	2.27	0.45
1:A:256:ASP:HB3	1:A:287:PHE:HA	1.99	0.45
1:B:6:PRO:HB2	4:B:1622:HOH:O	2.17	0.45
1:A:47:ALA:CA	1:A:306:MET:HE1	2.46	0.44
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.52	0.44
1:A:25:PHE:HB3	1:B:93:PHE:CD2	2.52	0.44
1:A:40:GLN:O	1:A:44:GLU:HG3	2.18	0.44
1:A:221:GLN:NE2	1:A:248:GLN:HB3	2.33	0.43
1:B:227:PHE:CZ	1:B:231:ILE:HD11	2.53	0.43
1:A:25:PHE:HB3	1:B:93:PHE:HD2	1.83	0.43
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.83	0.43
1:A:181:PRO:HA	4:A:1018:HOH:O	2.17	0.43
1:A:57:LEU:HD11	1:A:74:PHE:HB2	1.99	0.43
1:A:161:PHE:O	1:A:211:TYR:OH	2.34	0.43
1:A:231:ILE:HD13	1:A:231:ILE:HA	1.91	0.43
1:A:72:LYS:O	1:A:76:GLN:HG3	2.18	0.43
1:A:280:GLU:HG3	4:A:1606:HOH:O	2.17	0.43
1:B:17:VAL:HG21	1:B:38:THR:HG23	2.01	0.43
1:A:6:PRO:HA	4:A:1596:HOH:O	2.18	0.42
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.77	0.42
1:A:268:PHE:CD1	1:A:382:LEU:HD13	2.54	0.42
1:A:10:PHE:HB3	1:A:306:MET:HE3	2.02	0.42
1:A:87:MET:HA	1:A:132:THR:O	2.19	0.42
1:B:315:ARG:HD3	1:B:315:ARG:HA	1.80	0.42
1:B:2:TYR:N	4:B:1538:HOH:O	2.53	0.42
1:B:353:ARG:HA	1:B:357:GLU:OE1	2.20	0.41
1:A:286:ASP:OD2	3:A:960:HYA:H2	2.20	0.41
1:B:58:ILE:HA	1:B:59:PRO:HD3	1.80	0.41
1:A:139:ARG:NH1	1:A:186:PRO:HB2	2.35	0.41
1:B:202:ILE:HG23	1:B:211:TYR:HB2	2.02	0.41
1:B:87:MET:SD	1:B:88:ALA:N	2.94	0.41
1:A:116:ARG:NE	4:A:1635:HOH:O	2.46	0.41
1:B:184:ASN:HD22	1:B:185:GLU:HB2	1.86	0.41
1:A:12:PHE:HD1	4:A:1593:HOH:O	2.03	0.40

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	383/386 (99%)	367 (96%)	13 (3%)	3 (1%)	19	6
1	B	383/386 (99%)	367 (96%)	14 (4%)	2 (0%)	29	11
All	All	766/772 (99%)	734 (96%)	27 (4%)	5 (1%)	22	7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	ASP
1	B	344	ASP
1	A	185	GLU
1	B	185	GLU
1	A	23	ASP

### 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	301/302 (100%)	289 (96%)	12 (4%)	31	10
1	B	301/302 (100%)	287 (95%)	14 (5%)	26	7
All	All	602/604 (100%)	576 (96%)	26 (4%)	29	9

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	SER

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Mol	Chain	Res	Type
1	A	66	GLU
1	A	115	LEU
1	A	120	ARG
1	A	131	LYS
1	A	156	ARG
1	A	163	LEU
1	A	184	ASN
1	A	185	GLU
1	A	273	LEU
1	A	334	LEU
1	A	350	LEU
1	B	3	GLN
1	B	7	GLU
1	B	41	ARG
1	B	44	GLU
1	B	65	THR
1	B	66	GLU
1	B	163	LEU
1	B	184	ASN
1	B	185	GLU
1	B	199	LEU
1	B	204	ARG
1	B	206	GLU
1	B	347	GLN
1	B	361	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	214	ASN
1	A	221	GLN
1	A	308	ASN
1	A	326	GLN
1	A	339	GLN
1	B	76	GLN
1	B	95	HIS
1	B	184	ASN
1	B	221	GLN
1	B	308	ASN
1	B	347	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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
3	HYA	A	960	2	8,9,9	2.73	2 (25%)	4,11,11	2.35	2 (50%)
3	HYA	B	970	2	8,9,9	3.63	2 (25%)	4,11,11	1.60	1 (25%)

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
3	HYA	A	960	2	1/1/3/3	5/8/12/12	-
3	HYA	B	970	2	-	4/8/12/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	970	HYA	C1-N	8.61	1.35	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	960	HYA	C2-C1	5.35	1.54	1.49
3	B	970	HYA	C2-C1	5.04	1.54	1.49
3	A	960	HYA	C1-N	4.74	1.32	1.27

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	960	HYA	C4-C3-C2	3.92	118.75	111.95
3	B	970	HYA	C4-C3-C2	2.47	116.24	111.95
3	A	960	HYA	O3-C3-C4	-2.28	103.80	109.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	960	HYA	C2

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	960	HYA	C1-C2-C3-C4
3	A	960	HYA	C1-C2-C3-O3
3	A	960	HYA	O2-C2-C3-C4
3	A	960	HYA	O2-C2-C3-O3
3	B	970	HYA	O1-C1-C2-O2
3	A	960	HYA	O1-C1-C2-O2
3	B	970	HYA	O1-C1-C2-C3
3	B	970	HYA	C1-C2-C3-C4
3	B	970	HYA	O2-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	960	HYA	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	64:ASP	C	65:THR	N	1.90
1	A	149:ASP	C	150:VAL	N	1.12
1	A	63:SER	C	64:ASP	N	0.90

## 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.