



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:29 PM GMT

PDB ID : 1XIN  
Title : PROTEIN ENGINEERING OF XYLOSE (GLUCOSE) ISOMERASE FROM ACTINOPLANES MISSOURIENSIS. 1. CRYSTALLOGRAPHY AND SITE-DIRECTED MUTAGENESIS OF METAL BINDING SITES  
Authors : Janin, J.  
Deposited on : 1992-04-06  
Resolution : 2.40 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (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

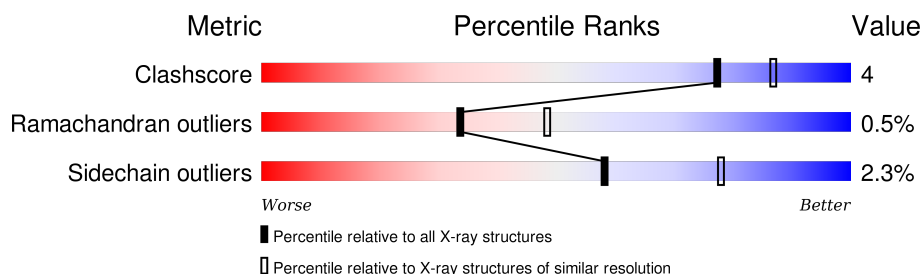
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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. 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  $\leq 5\%$ . 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	393	 80% 17% . .
1	B	393	 81% 16% .
1	C	393	 82% 15% .
1	D	393	 81% 16% .

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13137 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.

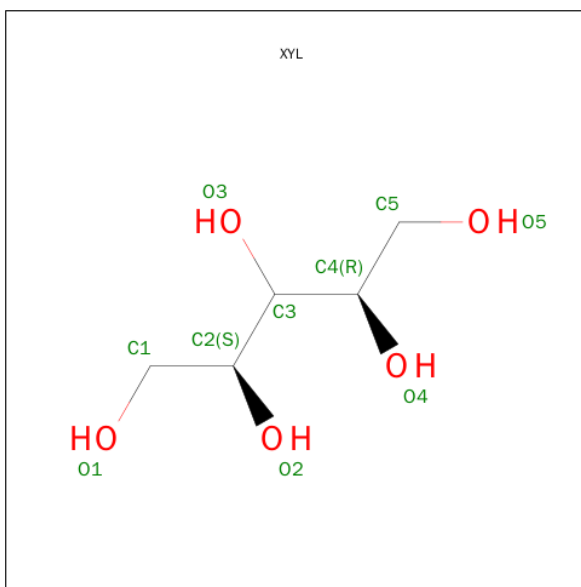
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3051	1937	531	579	4			
1	B	392	Total	C	N	O	S	0	0	0
			3051	1937	531	579	4			
1	C	392	Total	C	N	O	S	0	0	0
			3051	1937	531	579	4			
1	D	392	Total	C	N	O	S	0	0	0
			3051	1937	531	579	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	ASN	HIS	CONFLICT	UNP P12851
B	220	ASN	HIS	CONFLICT	UNP P12851
C	220	ASN	HIS	CONFLICT	UNP P12851
D	220	ASN	HIS	CONFLICT	UNP P12851

- Molecule 2 is SUGAR (D-XYLOSE (LINEAR FORM)) (three-letter code: XYL) (formula:  $C_5H_{12}O_5$ ).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	220	Total	O	0	0
			220	220		

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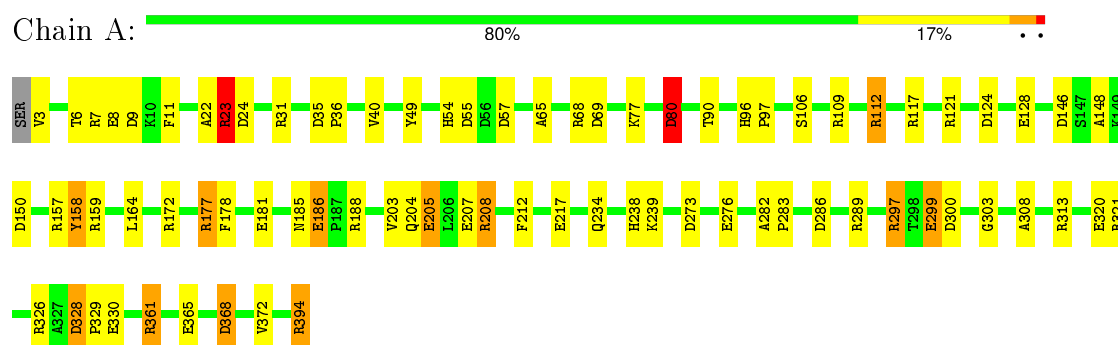
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	217	Total 217	O 217	0	0
4	C	232	Total 232	O 232	0	0
4	D	220	Total 220	O 220	0	0

### 3 Residue-property plots

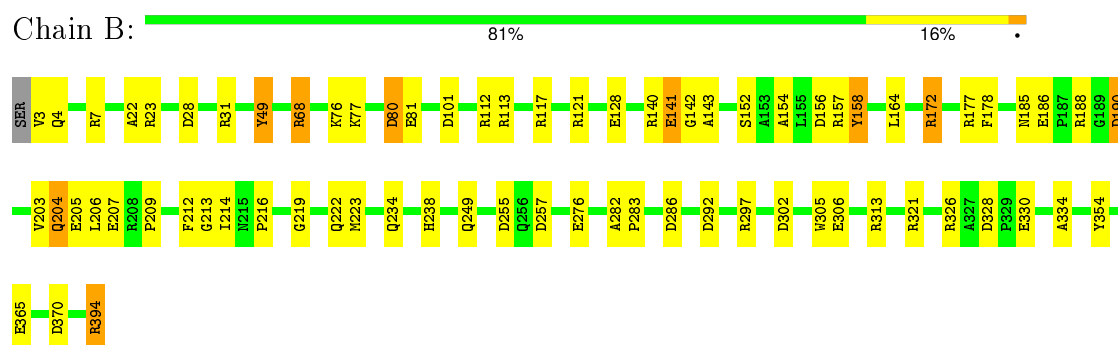
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

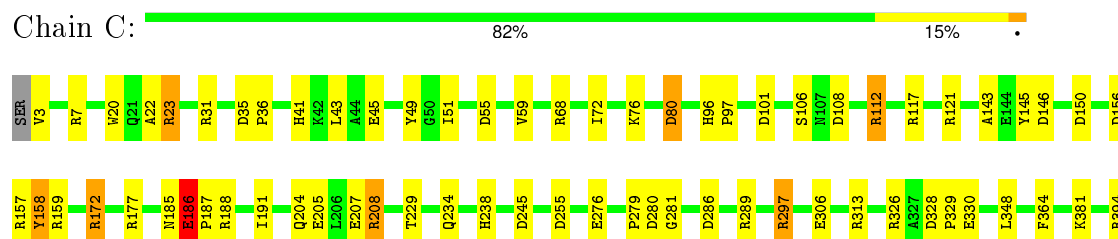
#### • Molecule 1: D-XYLOSE ISOMERASE



#### • Molecule 1: D-XYLOSE ISOMERASE

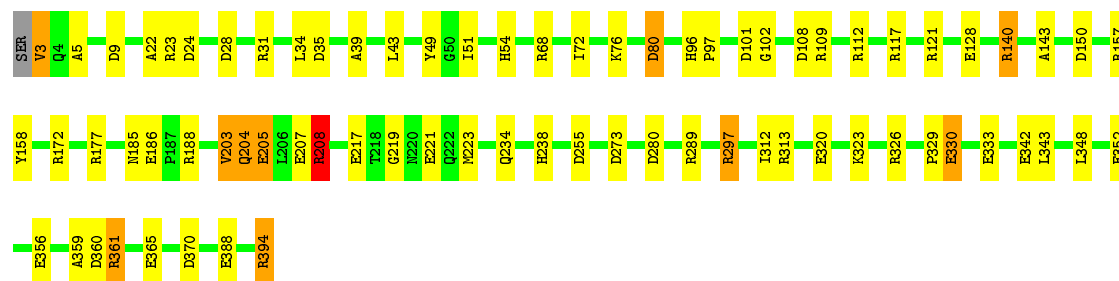


#### • Molecule 1: D-XYLOSE ISOMERASE



#### • Molecule 1: D-XYLOSE ISOMERASE

Chain D:



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.45Å 143.45Å 231.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.155 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13137	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: MG, XYZ

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	0.83	0/3122	1.75	71/4229 (1.7%)
1	B	0.83	0/3122	1.77	56/4229 (1.3%)
1	C	0.83	1/3122 (0.0%)	1.69	55/4229 (1.3%)
1	D	0.84	0/3122	1.74	58/4229 (1.4%)
All	All	0.83	1/12488 (0.0%)	1.74	240/16916 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	186	GLU	CD-OE2	-5.38	1.19	1.25

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	ARG	NE-CZ-NH1	20.25	130.42	120.30
1	B	172	ARG	NE-CZ-NH1	18.18	129.39	120.30
1	B	394	ARG	NE-CZ-NH2	-17.48	111.56	120.30
1	B	157	ARG	NE-CZ-NH1	15.69	128.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	ARG	NE-CZ-NH2	-15.12	112.74	120.30
1	C	117	ARG	NE-CZ-NH1	14.52	127.56	120.30
1	A	326	ARG	NE-CZ-NH1	14.32	127.46	120.30
1	C	172	ARG	NE-CZ-NH1	14.18	127.39	120.30
1	B	172	ARG	NE-CZ-NH2	-14.16	113.22	120.30
1	A	172	ARG	NE-CZ-NH1	13.48	127.04	120.30
1	D	117	ARG	NE-CZ-NH1	13.43	127.02	120.30
1	B	140	ARG	NE-CZ-NH2	-13.24	113.68	120.30
1	A	361	ARG	NE-CZ-NH1	12.84	126.72	120.30
1	D	150	ASP	CB-CG-OD1	12.71	129.74	118.30
1	C	172	ARG	NE-CZ-NH2	-12.28	114.16	120.30
1	D	140	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	A	394	ARG	NE-CZ-NH2	-12.07	114.26	120.30
1	D	255	ASP	CB-CG-OD2	-11.89	107.60	118.30
1	A	117	ARG	NE-CZ-NH1	11.79	126.19	120.30
1	C	177	ARG	NE-CZ-NH1	11.35	125.98	120.30
1	A	80	ASP	CB-CG-OD1	-11.35	108.08	118.30
1	A	321	ARG	NE-CZ-NH1	11.27	125.94	120.30
1	B	321	ARG	NE-CZ-NH2	-11.27	114.66	120.30
1	D	313	ARG	NE-CZ-NH2	11.24	125.92	120.30
1	C	158	TYR	CB-CG-CD2	11.15	127.69	121.00
1	B	177	ARG	NE-CZ-NH2	-11.15	114.72	120.30
1	B	113	ARG	NE-CZ-NH1	10.97	125.79	120.30
1	D	172	ARG	CD-NE-CZ	10.97	138.95	123.60
1	D	188	ARG	NE-CZ-NH2	10.92	125.76	120.30
1	B	68	ARG	NE-CZ-NH1	-10.80	114.90	120.30
1	B	157	ARG	NE-CZ-NH2	-10.49	115.05	120.30
1	A	328	ASP	CB-CG-OD2	10.44	127.69	118.30
1	A	205	GLU	OE1-CD-OE2	-10.04	111.25	123.30
1	C	188	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	D	255	ASP	CB-CG-OD1	9.91	127.22	118.30
1	B	158	TYR	CB-CG-CD2	9.88	126.93	121.00
1	C	297	ARG	NE-CZ-NH2	9.82	125.21	120.30
1	B	330	GLU	OE1-CD-OE2	9.78	135.03	123.30
1	A	172	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	A	326	ARG	NE-CZ-NH2	-9.53	115.53	120.30
1	A	150	ASP	CB-CG-OD1	9.46	126.81	118.30
1	A	7	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	D	117	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	A	146	ASP	CB-CG-OD1	9.26	126.64	118.30
1	B	286	ASP	CB-CG-OD1	9.21	126.59	118.30
1	D	326	ARG	NE-CZ-NH2	9.18	124.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A	117	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	A	172	ARG	CD-NE-CZ	8.93	136.10	123.60
1	D	35	ASP	CB-CG-OD1	8.88	126.29	118.30
1	D	330	GLU	OE1-CD-OE2	8.83	133.89	123.30
1	A	188	ARG	CD-NE-CZ	8.80	135.93	123.60
1	A	31	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	A	80	ASP	CA-CB-CG	-8.72	94.22	113.40
1	D	31	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	A	124	ASP	CB-CG-OD1	8.52	125.97	118.30
1	D	109	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	C	80	ASP	CB-CG-OD1	-8.47	110.68	118.30
1	A	121	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	A	158	TYR	CB-CG-CD2	8.39	126.03	121.00
1	C	117	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	B	31	ARG	NE-CZ-NH2	8.38	124.49	120.30
1	C	31	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	B	80	ASP	CB-CG-OD1	-8.29	110.84	118.30
1	A	394	ARG	NH1-CZ-NH2	8.29	128.51	119.40
1	B	113	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	C	23	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	D	9	ASP	CB-CG-OD2	8.13	125.62	118.30
1	D	24	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	C	23	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	D	370	ASP	CB-CG-OD2	8.00	125.50	118.30
1	A	273	ASP	CB-CG-OD1	7.98	125.48	118.30
1	D	121	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	B	302	ASP	CB-CG-OD1	7.97	125.47	118.30
1	C	186	GLU	OE1-CD-OE2	-7.85	113.88	123.30
1	B	112	ARG	NE-CZ-NH1	-7.77	116.41	120.30
1	D	9	ASP	CB-CG-OD1	-7.75	111.32	118.30
1	C	276	GLU	OE1-CD-OE2	-7.72	114.04	123.30
1	C	330	GLU	OE1-CD-OE2	7.71	132.55	123.30
1	C	313	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	300	ASP	CB-CG-OD1	7.66	125.20	118.30
1	B	156	ASP	CB-CG-OD2	-7.65	111.41	118.30
1	D	112	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	C	7	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	109	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	B	302	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	A	361	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	A	188	ARG	NE-CZ-NH2	7.51	124.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	ASP	CB-CG-OD2	7.40	124.96	118.30
1	B	158	TYR	CB-CG-CD1	-7.37	116.58	121.00
1	D	208	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	B	121	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	A	297	ARG	NE-CZ-NH2	7.35	123.97	120.30
1	A	80	ASP	OD1-CG-OD2	7.34	137.24	123.30
1	D	172	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	D	394	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	24	ASP	CB-CG-OD1	7.30	124.87	118.30
1	D	188	ARG	NE-CZ-NH1	-7.25	116.67	120.30
1	C	157	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	55	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	320	GLU	OE1-CD-OE2	-7.20	114.66	123.30
1	A	121	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	C	394	ARG	NE-CZ-NH1	-7.11	116.75	120.30
1	B	141	GLU	OE1-CD-OE2	-7.03	114.86	123.30
1	D	360	ASP	CB-CG-OD1	-6.99	112.01	118.30
1	C	286	ASP	CB-CG-OD1	6.97	124.57	118.30
1	A	68	ARG	CD-NE-CZ	6.96	133.34	123.60
1	B	394	ARG	N-CA-CB	6.96	123.12	110.60
1	B	321	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	D	109	ARG	CD-NE-CZ	6.94	133.32	123.60
1	C	313	ARG	CD-NE-CZ	6.93	133.30	123.60
1	A	68	ARG	NE-CZ-NH2	6.91	123.76	120.30
1	A	186	GLU	OE1-CD-OE2	-6.79	115.15	123.30
1	D	342	GLU	CG-CD-OE2	6.78	131.87	118.30
1	C	55	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	205	GLU	CG-CD-OE2	6.66	131.62	118.30
1	C	108	ASP	CB-CG-OD1	6.66	124.29	118.30
1	D	24	ASP	CB-CG-OD1	6.65	124.29	118.30
1	D	140	ARG	NH1-CZ-NH2	6.65	126.72	119.40
1	A	55	ASP	CB-CG-OD1	6.61	124.25	118.30
1	C	276	GLU	CG-CD-OE2	6.59	131.48	118.30
1	A	368	ASP	CB-CG-OD1	6.57	124.21	118.30
1	C	145	TYR	CB-CG-CD2	6.55	124.93	121.00
1	D	204	GLN	OE1-CD-NE2	-6.54	106.87	121.90
1	C	245	ASP	CB-CG-OD1	6.52	124.17	118.30
1	B	28	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	C	121	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	A	57	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	B	177	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	112	ARG	NE-CZ-NH1	-6.30	117.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	ASP	CB-CG-OD1	6.28	123.95	118.30
1	C	156	ASP	CB-CG-OD1	6.28	123.95	118.30
1	D	342	GLU	OE1-CD-OE2	-6.27	115.78	123.30
1	A	23	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	C	207	GLU	CG-CD-OE1	6.20	130.71	118.30
1	D	54	HIS	N-CA-CB	6.20	121.76	110.60
1	D	205	GLU	CG-CD-OE2	6.19	130.69	118.30
1	D	203	VAL	CA-CB-CG1	6.18	120.16	110.90
1	A	394	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	C	101	ASP	CB-CG-OD2	6.16	123.84	118.30
1	D	177	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	C	80	ASP	OD1-CG-OD2	6.14	134.97	123.30
1	C	177	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	297	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	A	394	ARG	CA-CB-CG	6.11	126.83	113.40
1	D	150	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	D	80	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	D	221	GLU	CG-CD-OE1	6.08	130.46	118.30
1	D	205	GLU	OE1-CD-OE2	-6.07	116.02	123.30
1	D	68	ARG	NE-CZ-NH2	6.05	123.32	120.30
1	C	208	ARG	CD-NE-CZ	-6.05	115.14	123.60
1	C	150	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	300	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	C	159	ARG	NE-CZ-NH1	-5.95	117.32	120.30
1	A	157	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	255	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	A	23	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	D	207	GLU	CA-CB-CG	5.89	126.37	113.40
1	B	204	GLN	OE1-CD-NE2	-5.85	108.44	121.90
1	C	177	ARG	N-CA-CB	5.85	121.14	110.60
1	A	158	TYR	CB-CG-CD1	-5.84	117.50	121.00
1	C	289	ARG	CD-NE-CZ	5.83	131.77	123.60
1	B	188	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	B	121	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	B	255	ASP	CB-CG-OD1	5.75	123.47	118.30
1	D	28	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	C	313	ARG	NH1-CZ-NH2	-5.74	113.09	119.40
1	A	31	ARG	NH1-CZ-NH2	5.74	125.71	119.40
1	D	333	GLU	CG-CD-OE2	5.74	129.77	118.30
1	C	281	GLY	N-CA-C	-5.73	98.77	113.10
1	C	207	GLU	CG-CD-OE2	-5.71	106.89	118.30
1	C	326	ARG	NE-CZ-NH2	5.70	123.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	143	ALA	N-CA-CB	-5.70	102.13	110.10
1	D	217	GLU	CG-CD-OE1	-5.68	106.93	118.30
1	A	289	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	299	GLU	OE1-CD-OE2	5.68	130.11	123.30
1	C	172	ARG	CD-NE-CZ	-5.65	115.69	123.60
1	D	157	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	C	158	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	C	45	GLU	CA-CB-CG	5.61	125.74	113.40
1	C	208	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	276	GLU	OE1-CD-OE2	-5.58	116.60	123.30
1	B	305	TRP	CA-CB-CG	-5.58	103.10	113.70
1	A	146	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	B	326	ARG	CD-NE-CZ	5.52	131.33	123.60
1	B	190	ASP	N-CA-CB	5.52	120.53	110.60
1	C	191	ILE	CA-CB-CG2	5.47	121.85	110.90
1	B	313	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	8	GLU	OE1-CD-OE2	5.46	129.85	123.30
1	B	112	ARG	CG-CD-NE	5.45	123.25	111.80
1	C	229	THR	CA-CB-OG1	-5.45	97.55	109.00
1	B	334	ALA	CB-CA-C	5.43	118.25	110.10
1	D	112	ARG	CD-NE-CZ	5.42	131.19	123.60
1	B	394	ARG	CD-NE-CZ	-5.42	116.01	123.60
1	D	289	ARG	CD-NE-CZ	5.41	131.17	123.60
1	D	361	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	A	181	GLU	CG-CD-OE1	5.40	129.10	118.30
1	A	217	GLU	CG-CD-OE2	5.40	129.10	118.30
1	D	320	GLU	CA-CB-CG	5.38	125.24	113.40
1	B	365	GLU	OE1-CD-OE2	-5.38	116.84	123.30
1	D	273	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	108	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	394	ARG	NH1-CZ-NH2	5.35	125.28	119.40
1	A	207	GLU	CA-CB-CG	5.34	125.14	113.40
1	C	255	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	D	388	GLU	CG-CD-OE2	5.33	128.96	118.30
1	A	177	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	306	GLU	CG-CD-OE1	5.32	128.94	118.30
1	B	68	ARG	NE-CZ-NH2	5.31	122.96	120.30
1	A	313	ARG	N-CA-CB	-5.30	101.05	110.60
1	B	330	GLU	CG-CD-OE2	-5.30	107.69	118.30
1	C	112	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	B	370	ASP	CB-CG-OD1	5.30	123.07	118.30
1	D	361	ARG	NE-CZ-NH1	-5.28	117.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	A	394	ARG	CD-NE-CZ	-5.27	116.22	123.60
1	B	394	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	68	ARG	NH1-CZ-NH2	-5.26	113.61	119.40
1	B	207	GLU	CG-CD-OE1	5.24	128.77	118.30
1	B	207	GLU	CG-CD-OE2	-5.23	107.84	118.30
1	B	257	ASP	CB-CG-OD2	5.23	123.00	118.30
1	D	101	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	143	ALA	CB-CA-C	-5.21	102.28	110.10
1	B	276	GLU	CG-CD-OE2	5.21	128.72	118.30
1	A	57	ASP	CB-CG-OD2	5.18	122.97	118.30
1	C	158	TYR	CA-CB-CG	5.18	123.24	113.40
1	C	145	TYR	CB-CG-CD1	-5.16	117.90	121.00
1	D	297	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	B	292	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	A	321	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	308	ALA	CB-CA-C	5.11	117.77	110.10
1	D	128	GLU	CA-CB-CG	5.11	124.64	113.40
1	A	8	GLU	CA-CB-CG	-5.10	102.19	113.40
1	A	148	ALA	N-CA-CB	-5.09	102.98	110.10
1	A	159	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	D	54	HIS	N-CA-C	-5.07	97.32	111.00
1	B	213	GLY	O-C-N	5.06	130.80	122.70
1	A	128	GLU	CG-CD-OE1	-5.04	108.22	118.30
1	B	143	ALA	N-CA-CB	-5.03	103.06	110.10
1	A	208	ARG	CA-CB-CG	5.01	124.42	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	ARG	Sidechain
1	B	172	ARG	Sidechain
1	C	172	ARG	Sidechain
1	D	208	ARG	Sidechain

## 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	3051	0	2953	26	0
1	B	3051	0	2953	28	0
1	C	3051	0	2953	21	0
1	D	3051	0	2953	24	0
2	A	10	0	12	0	0
2	B	10	0	12	1	0
2	C	10	0	11	1	0
2	D	10	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	220	0	0	1	0
4	B	217	0	0	2	0
4	C	232	0	0	2	0
4	D	220	0	0	4	0
All	All	13137	0	11859	89	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 4.

All (89) 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:204:GLN:OE1	1:C:204:GLN:OE1	1.65	1.13
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.70	1.08
1:D:208:ARG:HH11	1:D:208:ARG:HG2	1.27	1.00
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.18	0.92
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.19	0.87
1:D:3:VAL:HG23	4:D:601:HOH:O	1.76	0.84
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.21	0.84
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.25	0.83
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.67	0.76
1:D:330:GLU:OE1	4:D:613:HOH:O	2.11	0.68
1:B:141:GLU:OE2	4:B:569:HOH:O	2.14	0.65
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.79	0.64
1:A:36:PRO:O	1:A:40:VAL:HG23	1.97	0.63
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.82	0.63
2:B:397:XYL:H12	4:B:593:HOH:O	1.99	0.62
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.83	0.61
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.85	0.59
1:D:208:ARG:NH1	1:D:208:ARG:HG2	2.03	0.58
2:C:397:XYL:H12	4:C:609:HOH:O	2.02	0.58
1:A:204:GLN:HG2	4:A:548:HOH:O	2.02	0.58
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.85	0.57
1:C:59:VAL:HG11	1:C:68:ARG:HG3	1.87	0.56
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.89	0.55
1:C:72:ILE:O	1:C:76:LYS:HG3	2.06	0.55
1:D:43:LEU:HD12	1:D:51:ILE:HD12	1.87	0.54
1:B:77:LYS:O	1:B:80:ASP:HB2	2.08	0.53
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.10	0.53
1:C:41:HIS:HE1	4:C:522:HOH:O	1.91	0.52
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.91	0.51
1:C:43:LEU:HD12	1:C:51:ILE:HD12	1.92	0.51
1:B:3:VAL:HG12	1:B:4:GLN:H	1.76	0.50
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.94	0.49
1:B:68:ARG:HH11	1:B:68:ARG:HG2	1.78	0.49
1:A:6:THR:O	1:A:9:ASP:HB2	2.13	0.49
1:B:203:VAL:HG22	1:B:212:PHE:HB3	1.95	0.49
1:D:102:GLY:HA2	1:D:140:ARG:HB2	1.95	0.48
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.48	0.48
1:A:65:ALA:O	1:A:69:ASP:HB2	2.13	0.48
1:D:5:ALA:HB2	1:D:312:ILE:HG21	1.95	0.48
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.48	0.48
1:B:22:ALA:HB1	1:B:297:ARG:HG3	1.94	0.48
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.49	0.47
1:A:23:ARG:HG2	1:B:23:ARG:NH1	2.29	0.47
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.74	0.47
1:C:106:SER:O	1:C:112:ARG:HD3	2.15	0.47
1:D:361:ARG:HB3	1:D:365:GLU:HB2	1.96	0.46
1:C:328:ASP:HA	1:C:329:PRO:HD3	1.76	0.46
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.92	0.46
1:C:208:ARG:HD3	1:C:208:ARG:HH11	1.50	0.45
1:A:238:HIS:O	1:A:239:LYS:HB2	2.15	0.45
1:A:368:ASP:O	1:A:372:VAL:HG23	2.17	0.45
1:B:164:LEU:C	1:B:164:LEU:HD23	2.37	0.44
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.71	0.44
1:A:77:LYS:O	1:A:80:ASP:CB	2.65	0.44
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.13	0.44
1:B:219:GLY:O	1:B:223:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.89	0.44
1:A:299:GLU:HB3	1:A:303:GLY:HA3	2.00	0.43
1:C:20:TRP:CE2	1:C:22:ALA:HA	2.54	0.42
1:B:178:PHE:HB2	1:B:212:PHE:CD2	2.54	0.42
1:A:35:ASP:HA	1:A:36:PRO:HD3	1.84	0.42
1:B:142:GLY:HA3	1:B:190:ASP:O	2.18	0.42
1:A:164:LEU:HD12	1:C:348:LEU:HD11	2.00	0.42
1:C:186:GLU:HA	1:C:187:PRO:HA	1.91	0.42
1:D:356:GLU:O	1:D:359:ALA:HB3	2.19	0.42
1:B:282:ALA:HB1	1:B:283:PRO:HD2	2.01	0.42
1:C:23:ARG:CZ	1:D:23:ARG:HD2	2.50	0.42
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.89	0.42
1:A:330:GLU:OE1	1:A:394:ARG:NH1	2.52	0.42
1:B:7:ARG:HG2	1:B:49:TYR:HB2	2.02	0.42
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.87	0.41
1:C:59:VAL:HG21	1:C:68:ARG:HG3	2.02	0.41
1:D:22:ALA:HB1	1:D:297:ARG:HG3	2.02	0.41
1:B:206:LEU:O	1:B:209:PRO:HD3	2.19	0.41
1:B:152:SER:HB2	4:D:572:HOH:O	2.20	0.41
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.86	0.41
1:B:101:ASP:CG	1:B:101:ASP:O	2.58	0.41
1:B:76:LYS:NZ	1:B:128:GLU:OE2	2.46	0.41
1:D:219:GLY:O	1:D:223:MET:HG3	2.20	0.41
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.20	0.41
1:D:72:ILE:O	1:D:76:LYS:HG3	2.21	0.41
1:D:34:LEU:CD2	1:D:39:ALA:HB2	2.51	0.41
1:A:106:SER:O	1:A:112:ARG:HD3	2.21	0.41
1:A:164:LEU:HD23	1:A:164:LEU:C	2.41	0.40
1:B:214:ILE:HG13	1:B:216:PRO:HD3	2.03	0.40
1:B:68:ARG:HG2	1:B:68:ARG:NH1	2.36	0.40
1:D:394:ARG:NH1	4:D:609:HOH:O	1.96	0.40
1:A:178:PHE:HB2	1:A:212:PHE:CD2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	46	63
1	B	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	46	63
1	C	390/393 (99%)	374 (96%)	12 (3%)	4 (1%)	19	28
1	D	390/393 (99%)	378 (97%)	10 (3%)	2 (0%)	34	48
All	All	1560/1572 (99%)	1504 (96%)	48 (3%)	8 (0%)	34	48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	280	ASP
1	A	186	GLU
1	B	186	GLU
1	C	186	GLU
1	C	279	PRO
1	D	186	GLU
1	D	280	ASP
1	C	364	PHE

### 5.3.2 Protein sidechains ⓘ

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	306/310 (99%)	297 (97%)	9 (3%)	50	71
1	B	306/310 (99%)	301 (98%)	5 (2%)	70	86
1	C	306/310 (99%)	301 (98%)	5 (2%)	70	86
1	D	306/310 (99%)	297 (97%)	9 (3%)	50	71
All	All	1224/1240 (99%)	1196 (98%)	28 (2%)	58	78

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	49	TYR
1	A	80	ASP
1	A	158	TYR
1	A	177	ARG
1	A	185	ASN
1	A	203	VAL
1	A	208	ARG
1	A	286	ASP
1	B	49	TYR
1	B	81	GLU
1	B	158	TYR
1	B	185	ASN
1	B	394	ARG
1	C	3	VAL
1	C	49	TYR
1	C	80	ASP
1	C	158	TYR
1	C	185	ASN
1	D	3	VAL
1	D	49	TYR
1	D	80	ASP
1	D	158	TYR
1	D	185	ASN
1	D	203	VAL
1	D	208	ARG
1	D	323	LYS
1	D	329	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	A	204	GLN
1	A	238	HIS
1	B	204	GLN
1	B	238	HIS
1	C	41	HIS
1	C	185	ASN
1	C	222	GLN
1	C	238	HIS
1	D	185	ASN
1	D	238	HIS

### 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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	397	3	9,9,9	0.51	0	10,11,11	1.43	1 (10%)
2	XYL	B	397	3	9,9,9	0.47	0	10,11,11	2.28	3 (30%)
2	XYL	C	397	3	9,9,9	0.53	0	10,11,11	1.67	2 (20%)
2	XYL	D	397	3	9,9,9	0.53	0	10,11,11	1.72	3 (30%)

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	397	3	-	0/12/12/12	0/0/0/0
2	XYL	B	397	3	-	0/12/12/12	0/0/0/0
2	XYL	C	397	3	-	0/12/12/12	0/0/0/0
2	XYL	D	397	3	-	0/12/12/12	0/0/0/0

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	XYL	O2-C2-C3	-2.22	103.44	109.02
2	D	397	XYL	O2-C2-C1	-2.05	104.44	109.22
2	D	397	XYL	C1-C2-C3	2.68	118.77	112.48
2	C	397	XYL	C1-C2-C3	2.92	119.34	112.48
2	D	397	XYL	C5-C4-C3	3.45	120.56	112.48
2	C	397	XYL	O4-C4-C3	3.60	118.07	109.02
2	A	397	XYL	O4-C4-C3	3.67	118.25	109.02
2	B	397	XYL	C1-C2-C3	4.20	122.32	112.48
2	B	397	XYL	O4-C4-C3	4.69	120.80	109.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	397	XYL	1	0
2	C	397	XYL	1	0

## 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 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.