



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 07:17 AM BST

PDB ID : 5XIN  
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 : 2.30 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) : 2.13.1

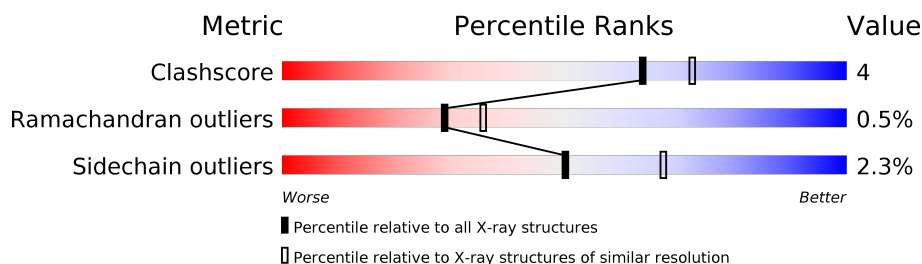
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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	393	
1	B	393	
1	C	393	
1	D	393	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13125 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.

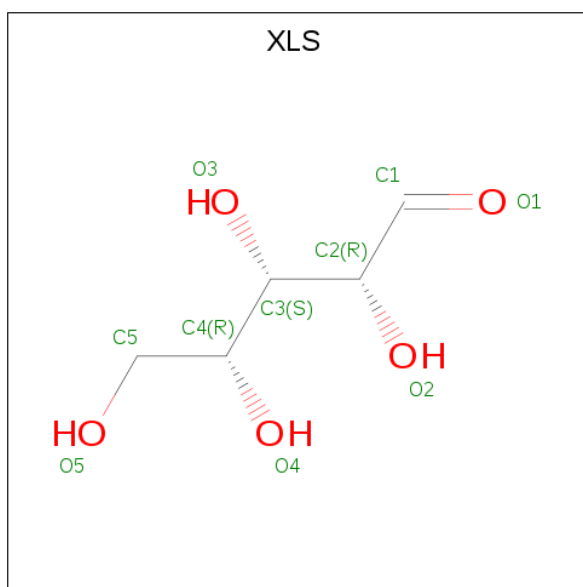
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3050	1938	532	576	4			
1	B	392	Total	C	N	O	S	0	0	0
			3050	1938	532	576	4			
1	C	392	Total	C	N	O	S	0	0	0
			3050	1938	532	576	4			
1	D	392	Total	C	N	O	S	0	0	0
			3050	1938	532	576	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	ALA	ASP	conflict	UNP P12851
B	255	ALA	ASP	conflict	UNP P12851
C	255	ALA	ASP	conflict	UNP P12851
D	255	ALA	ASP	conflict	UNP P12851

- Molecule 2 is D-xylose (three-letter code: XLS) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).



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	224	Total	O	0	0
			224	224		

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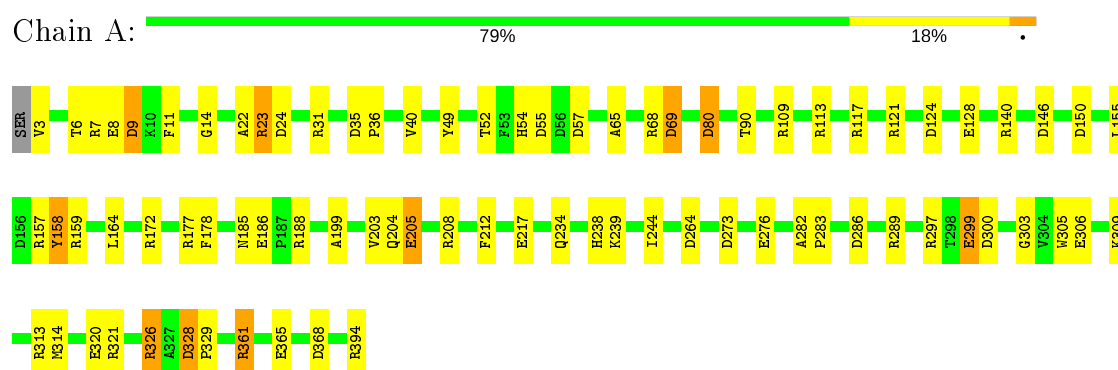
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	214	Total 214	O 214	0	0
4	C	232	Total 232	O 232	0	0
4	D	211	Total 211	O 211	0	0

### 3 Residue-property plots [i](#)

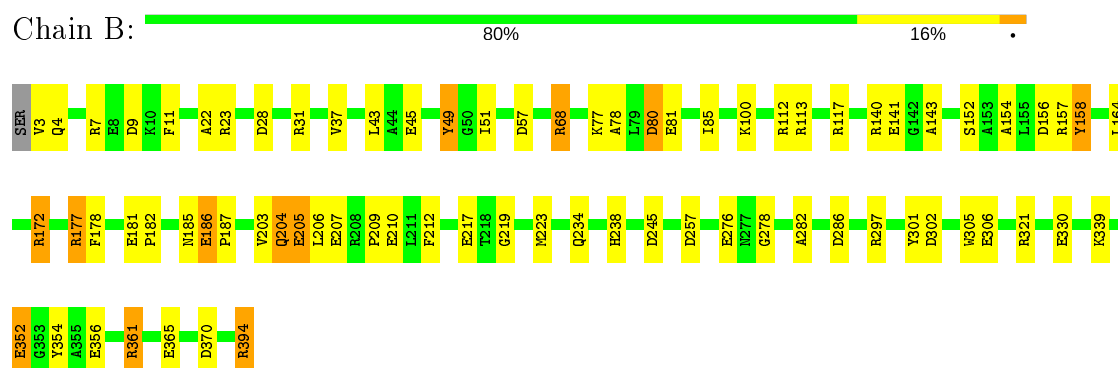
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

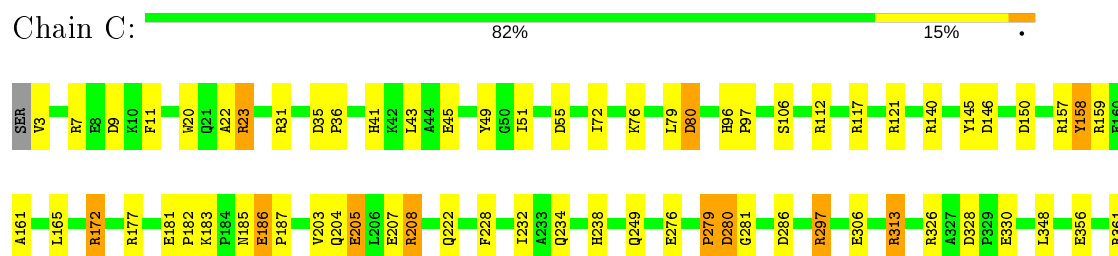
#### • Molecule 1: D-XYLOSE ISOMERASE



#### • Molecule 1: D-XYLOSE ISOMERASE

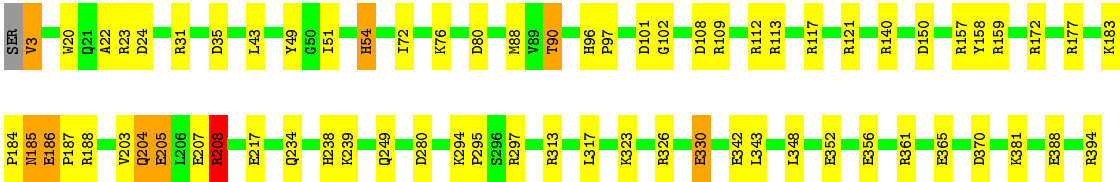
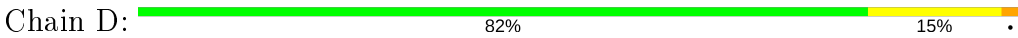


#### • Molecule 1: D-XYLOSE ISOMERASE





● 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	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) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.152 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, XLS

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	0.82	0/3122	1.68	62/4229 (1.5%)
1	B	0.81	0/3122	1.67	50/4229 (1.2%)
1	C	0.81	0/3122	1.67	51/4229 (1.2%)
1	D	0.82	0/3122	1.64	46/4229 (1.1%)
All	All	0.82	0/12488	1.66	209/16916 (1.2%)

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	2
1	C	0	1
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	ARG	NE-CZ-NH1	18.50	129.55	120.30
1	B	172	ARG	NE-CZ-NH2	-16.88	111.86	120.30
1	C	172	ARG	NE-CZ-NH2	-16.78	111.91	120.30
1	B	177	ARG	NE-CZ-NH2	-16.30	112.15	120.30
1	B	117	ARG	NE-CZ-NH1	16.27	128.43	120.30
1	C	117	ARG	NE-CZ-NH1	15.13	127.86	120.30
1	B	394	ARG	NE-CZ-NH2	-14.51	113.05	120.30
1	C	172	ARG	NE-CZ-NH1	14.44	127.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	117	ARG	NE-CZ-NH1	14.34	127.47	120.30
1	C	177	ARG	NE-CZ-NH1	13.13	126.87	120.30
1	A	326	ARG	NE-CZ-NH1	12.39	126.50	120.30
1	A	172	ARG	NE-CZ-NH1	12.38	126.49	120.30
1	A	394	ARG	NE-CZ-NH2	-12.34	114.13	120.30
1	B	117	ARG	NE-CZ-NH2	-12.33	114.14	120.30
1	A	80	ASP	CB-CG-OD1	-11.61	107.85	118.30
1	A	361	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	C	121	ARG	NE-CZ-NH1	11.49	126.05	120.30
1	D	121	ARG	NE-CZ-NH2	-11.28	114.66	120.30
1	D	150	ASP	CB-CG-OD1	11.18	128.36	118.30
1	A	121	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	A	321	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	D	313	ARG	NE-CZ-NH2	10.62	125.61	120.30
1	A	146	ASP	CB-CG-OD1	10.57	127.81	118.30
1	A	205	GLU	OE1-CD-OE2	-10.50	110.70	123.30
1	B	158	TYR	CB-CG-CD2	10.19	127.11	121.00
1	B	330	GLU	OE1-CD-OE2	10.11	135.43	123.30
1	D	109	ARG	NE-CZ-NH1	10.07	125.34	120.30
1	B	113	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	D	117	ARG	NE-CZ-NH2	-9.96	115.32	120.30
1	B	177	ARG	NE-CZ-NH1	9.91	125.26	120.30
1	D	172	ARG	CD-NE-CZ	9.89	137.45	123.60
1	C	313	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	A	23	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	A	328	ASP	CB-CG-OD2	9.54	126.89	118.30
1	C	23	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	D	35	ASP	CB-CG-OD1	9.42	126.78	118.30
1	A	117	ARG	NE-CZ-NH1	9.37	124.99	120.30
1	A	394	ARG	NH1-CZ-NH2	9.37	129.70	119.40
1	C	157	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	B	157	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	A	158	TYR	CB-CG-CD2	9.16	126.50	121.00
1	C	177	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	B	286	ASP	CB-CG-OD1	9.07	126.47	118.30
1	B	302	ASP	CB-CG-OD2	-9.01	110.20	118.30
1	B	156	ASP	CB-CG-OD2	-8.86	110.33	118.30
1	C	80	ASP	CB-CG-OD1	-8.80	110.38	118.30
1	A	157	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	C	158	TYR	CB-CG-CD2	8.74	126.25	121.00
1	D	342	GLU	OE1-CD-OE2	-8.57	113.01	123.30
1	B	112	ARG	NE-CZ-NH1	-8.57	116.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	297	ARG	NE-CZ-NH1	-8.56	116.02	120.30
1	B	321	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	A	68	ARG	NE-CZ-NH2	8.32	124.46	120.30
1	A	394	ARG	NE-CZ-NH1	-8.29	116.16	120.30
1	C	276	GLU	OE1-CD-OE2	-8.26	113.39	123.30
1	C	159	ARG	NE-CZ-NH1	-8.24	116.18	120.30
1	D	330	GLU	OE1-CD-OE2	8.19	133.13	123.30
1	A	150	ASP	CB-CG-OD1	8.15	125.64	118.30
1	A	113	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	D	342	GLU	CG-CD-OE2	8.12	134.55	118.30
1	D	188	ARG	NE-CZ-NH2	8.07	124.34	120.30
1	C	145	TYR	CB-CG-CD2	7.93	125.76	121.00
1	A	117	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	B	321	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	A	57	ASP	CB-CG-OD1	-7.83	111.26	118.30
1	A	199	ALA	CB-CA-C	7.73	121.70	110.10
1	C	208	ARG	NE-CZ-NH1	-7.73	116.44	120.30
1	B	80	ASP	CB-CG-OD1	-7.73	111.34	118.30
1	B	394	ARG	N-CA-CB	7.70	124.45	110.60
1	A	394	ARG	CA-CB-CG	7.62	130.16	113.40
1	D	208	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	273	ASP	CB-CG-OD1	7.52	125.07	118.30
1	B	31	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	B	68	ARG	NE-CZ-NH1	-7.45	116.58	120.30
1	C	23	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	80	ASP	CA-CB-CG	-7.42	97.08	113.40
1	A	326	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	D	113	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	B	140	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	D	109	ARG	CD-NE-CZ	7.29	133.81	123.60
1	A	300	ASP	CB-CG-OD1	7.28	124.85	118.30
1	C	326	ARG	NE-CZ-NH2	7.27	123.94	120.30
1	C	55	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	140	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	31	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	C	361	ARG	NE-CZ-NH2	7.14	123.87	120.30
1	C	177	ARG	N-CA-CB	7.10	123.39	110.60
1	A	159	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	B	158	TYR	CB-CG-CD1	-7.06	116.77	121.00
1	A	124	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	158	TYR	CB-CG-CD1	-6.93	116.84	121.00
1	D	370	ASP	CB-CG-OD2	6.90	124.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	297	ARG	NE-CZ-NH1	-6.88	116.86	120.30
1	D	109	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	188	ARG	CD-NE-CZ	6.82	133.15	123.60
1	B	302	ASP	CB-CG-OD1	6.80	124.42	118.30
1	C	145	TYR	CB-CG-CD1	-6.73	116.96	121.00
1	C	140	ARG	CD-NE-CZ	6.70	132.98	123.60
1	D	24	ASP	CB-CG-OD2	-6.67	112.29	118.30
1	A	121	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	D	204	GLN	OE1-CD-NE2	-6.65	106.61	121.90
1	A	172	ARG	CD-NE-CZ	6.63	132.88	123.60
1	C	172	ARG	CD-NE-CZ	-6.62	114.34	123.60
1	C	286	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	109	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	299	GLU	OE1-CD-OE2	6.53	131.13	123.30
1	B	361	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	C	208	ARG	CD-NE-CZ	-6.51	114.49	123.60
1	A	205	GLU	CG-CD-OE2	6.48	131.27	118.30
1	D	150	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	C	276	GLU	CG-CD-OE2	6.45	131.20	118.30
1	A	7	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	23	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	C	313	ARG	CD-NE-CZ	6.42	132.58	123.60
1	C	313	ARG	NH1-CZ-NH2	-6.39	112.37	119.40
1	B	352	GLU	OE1-CD-OE2	6.38	130.95	123.30
1	D	172	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	257	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	157	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	D	88	MET	CA-CB-CG	6.29	123.99	113.30
1	A	368	ASP	CB-CG-OD1	6.24	123.92	118.30
1	D	205	GLU	OE1-CD-OE2	-6.24	115.81	123.30
1	A	68	ARG	CD-NE-CZ	6.24	132.34	123.60
1	C	326	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	D	24	ASP	CB-CG-OD1	6.21	123.89	118.30
1	C	150	ASP	CB-CG-OD1	6.19	123.87	118.30
1	C	207	GLU	CG-CD-OE2	-6.12	106.06	118.30
1	D	205	GLU	CG-CD-OE2	6.12	130.54	118.30
1	B	28	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	C	45	GLU	CA-CB-CG	6.07	126.76	113.40
1	A	146	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	55	ASP	CB-CG-OD1	6.01	123.71	118.30
1	D	112	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	207	GLU	CA-CB-CG	5.99	126.58	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	C	297	ARG	NE-CZ-NH2	5.99	123.30	120.30
1	A	276	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	A	24	ASP	CB-CG-OD1	5.94	123.65	118.30
1	C	328	ASP	CB-CG-OD2	5.94	123.64	118.30
1	C	330	GLU	OE1-CD-OE2	5.93	130.41	123.30
1	A	80	ASP	OD1-CG-OD2	5.88	134.47	123.30
1	A	320	GLU	OE1-CD-OE2	-5.86	116.27	123.30
1	C	7	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	D	31	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	156	ASP	CB-CG-OD1	5.81	123.53	118.30
1	D	112	ARG	CD-NE-CZ	5.79	131.70	123.60
1	B	394	ARG	CD-NE-CZ	-5.78	115.51	123.60
1	C	207	GLU	CG-CD-OE1	5.77	129.85	118.30
1	B	204	GLN	OE1-CD-NE2	-5.75	108.68	121.90
1	D	121	ARG	NH1-CZ-NH2	5.74	125.71	119.40
1	B	361	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	370	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	305	TRP	CA-CB-CG	-5.64	102.97	113.70
1	C	356	GLU	OE1-CD-OE2	-5.63	116.54	123.30
1	A	23	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	D	159	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	306	GLU	CG-CD-OE1	5.60	129.50	118.30
1	C	146	ASP	CB-CG-OD1	5.55	123.29	118.30
1	B	330	GLU	CG-CD-OE2	-5.54	107.21	118.30
1	D	101	ASP	CB-CG-OD2	5.54	123.29	118.30
1	D	108	ASP	CB-CG-OD1	5.52	123.27	118.30
1	D	54	HIS	N-CA-CB	5.52	120.53	110.60
1	A	361	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	C	31	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	C	205	GLU	OE1-CD-OE2	-5.45	116.76	123.30
1	C	281	GLY	N-CA-C	-5.44	99.51	113.10
1	D	177	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	354	TYR	CB-CG-CD1	-5.41	117.75	121.00
1	B	141	GLU	OE1-CD-OE2	-5.40	116.83	123.30
1	D	208	ARG	CG-CD-NE	5.40	123.13	111.80
1	B	210	GLU	CA-CB-CG	5.38	125.23	113.40
1	A	155	LEU	CB-CA-C	5.37	120.40	110.20
1	B	45	GLU	CA-CB-CG	5.36	125.18	113.40
1	A	289	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	C	80	ASP	OD1-CG-OD2	5.31	133.39	123.30
1	B	276	GLU	CG-CD-OE2	5.31	128.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	GLU	CG-CD-OE2	5.29	128.88	118.30
1	C	306	GLU	CG-CD-OE2	-5.28	107.75	118.30
1	D	249	GLN	CA-CB-CG	5.25	124.95	113.40
1	C	117	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	69	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	A	9	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	207	GLU	CG-CD-OE1	5.22	128.74	118.30
1	D	326	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	D	90	THR	CA-CB-CG2	5.19	119.67	112.40
1	B	301	TYR	CB-CG-CD1	-5.19	117.89	121.00
1	C	205	GLU	CG-CD-OE2	5.18	128.66	118.30
1	C	150	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	57	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	140	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	394	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	B	143	ALA	N-CA-CB	-5.13	102.92	110.10
1	D	388	GLU	CG-CD-OE1	-5.12	108.06	118.30
1	B	205	GLU	CG-CD-OE2	5.12	128.54	118.30
1	D	207	GLU	CG-CD-OE1	5.12	128.53	118.30
1	D	157	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	394	ARG	CG-CD-NE	-5.11	101.08	111.80
1	A	8	GLU	OE1-CD-OE2	5.09	129.41	123.30
1	A	244	ILE	O-C-N	5.09	130.85	122.70
1	B	339	LYS	CD-CE-NZ	-5.09	100.00	111.70
1	C	121	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	128	GLU	CG-CD-OE1	-5.08	108.14	118.30
1	B	394	ARG	NH1-CZ-NH2	5.08	124.98	119.40
1	D	388	GLU	CG-CD-OE2	5.07	128.45	118.30
1	A	314	MET	CG-SD-CE	5.06	108.30	100.20
1	A	313	ARG	N-CA-CB	-5.05	101.52	110.60
1	D	217	GLU	CG-CD-OE1	-5.02	108.25	118.30
1	A	264	ASP	CB-CA-C	5.01	120.42	110.40
1	D	54	HIS	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	ARG	Sidechain
1	B	172	ARG	Sidechain
1	B	177	ARG	Sidechain
1	C	172	ARG	Sidechain

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Mol	Chain	Res	Type	Group
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	3050	0	2955	25	0
1	B	3050	0	2955	29	0
1	C	3050	0	2955	27	0
1	D	3050	0	2955	31	0
2	A	10	0	10	0	0
2	B	10	0	9	0	0
2	C	10	0	9	0	0
2	D	10	0	10	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	224	0	0	1	0
4	B	214	0	0	1	0
4	C	232	0	0	1	0
4	D	211	0	0	6	0
All	All	13125	0	11858	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 4.

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:204:GLN:OE1	1:C:204:GLN:OE1	1.61	1.19
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.61	1.18
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.10	0.96
1:D:208:ARG:HH11	1:D:208:ARG:HG2	1.33	0.94
1:D:3:VAL:HG23	4:D:594:HOH:O	1.73	0.86
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.20	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.22	0.85
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.25	0.82
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.66	0.76
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.02	0.74
1:A:204:GLN:HG2	4:A:551:HOH:O	1.92	0.70
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.74	0.68
1:D:330:GLU:OE1	4:D:606:HOH:O	2.13	0.65
1:D:394:ARG:NH1	4:D:603:HOH:O	2.16	0.60
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.83	0.60
1:C:228:PHE:CZ	1:C:232:ILE:HD11	2.37	0.59
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.84	0.59
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.85	0.59
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.85	0.59
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.85	0.58
1:B:7:ARG:HG2	1:B:49:TYR:HB2	1.85	0.57
1:C:43:LEU:HD12	1:C:51:ILE:HD12	1.88	0.55
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.89	0.55
1:A:65:ALA:O	1:A:69:ASP:HB2	2.07	0.54
1:D:43:LEU:HD12	1:D:51:ILE:HD12	1.88	0.54
1:B:203:VAL:HG22	1:B:212:PHE:HB3	1.90	0.53
1:A:238:HIS:O	1:A:239:LYS:HB2	2.08	0.53
1:C:183:LYS:HE2	1:C:185:ASN:O	2.10	0.52
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.45	0.51
1:D:208:ARG:NH1	1:D:208:ARG:HG2	2.09	0.51
1:A:36:PRO:O	1:A:40:VAL:HG23	2.11	0.51
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.93	0.51
1:B:77:LYS:O	1:B:80:ASP:HB2	2.11	0.50
1:A:306:GLU:HG2	1:D:381:LYS:HB2	1.93	0.50
1:C:72:ILE:O	1:C:76:LYS:HG3	2.12	0.49
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.47	0.49
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.47	0.49
1:C:228:PHE:CE1	1:C:232:ILE:HD11	2.48	0.48
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.94	0.48
1:C:41:HIS:HE1	4:C:521:HOH:O	1.96	0.48
1:D:238:HIS:O	1:D:239:LYS:HB2	2.13	0.47
1:D:54:HIS:CD2	1:D:90:THR:HG23	2.49	0.47
1:B:43:LEU:HD12	1:B:51:ILE:HD12	1.95	0.46
1:B:37:VAL:HG13	1:B:78:ALA:HB2	1.98	0.46
1:A:299:GLU:HB3	1:A:303:GLY:HA3	1.96	0.46
1:B:68:ARG:HH11	1:B:68:ARG:HG2	1.81	0.45
1:D:72:ILE:O	1:D:76:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.93	0.45
1:B:219:GLY:O	1:B:223:MET:HG3	2.17	0.45
1:D:3:VAL:CB	4:D:594:HOH:O	2.65	0.44
1:D:3:VAL:CG2	4:D:594:HOH:O	2.47	0.44
1:C:181:GLU:HA	1:C:182:PRO:HD3	1.87	0.44
1:B:181:GLU:HA	1:B:182:PRO:HD3	1.90	0.44
1:D:361:ARG:HB3	1:D:365:GLU:HB2	1.99	0.44
1:A:164:LEU:HD12	1:C:348:LEU:HD11	2.00	0.44
1:B:3:VAL:HG12	1:B:4:GLN:H	1.82	0.44
1:C:20:TRP:CE2	1:C:22:ALA:HA	2.53	0.44
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.78	0.43
1:C:23:ARG:CZ	1:D:23:ARG:HD2	2.49	0.43
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.90	0.43
1:D:102:GLY:HA2	1:D:140:ARG:HB2	2.00	0.43
1:A:305:TRP:O	1:A:309:LYS:HG3	2.19	0.43
1:B:9:ASP:HB3	1:B:11:PHE:CE2	2.54	0.43
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.19	0.43
1:D:317:LEU:HA	1:D:317:LEU:HD23	1.84	0.42
1:A:6:THR:O	1:A:9:ASP:HB2	2.20	0.42
1:A:234:GLN:HE21	1:A:238:HIS:CE1	2.13	0.42
1:B:352:GLU:HG2	1:B:356:GLU:HB2	2.00	0.42
1:C:186:GLU:HA	1:C:187:PRO:HA	1.92	0.42
1:C:222:GLN:HE21	1:C:249:GLN:HB3	1.83	0.42
1:D:186:GLU:HA	1:D:187:PRO:HA	1.80	0.42
1:D:294:LYS:HA	1:D:295:PRO:HD3	1.88	0.42
1:D:185:ASN:HD22	1:D:186:GLU:HB2	1.84	0.42
1:B:278:GLY:CA	1:B:282:ALA:O	2.68	0.42
1:C:106:SER:O	1:C:112:ARG:HD3	2.19	0.42
1:D:183:LYS:HG2	1:D:184:PRO:HD2	2.02	0.42
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.88	0.42
1:A:326:ARG:HA	1:A:326:ARG:HD3	1.89	0.42
1:B:22:ALA:HB1	1:B:297:ARG:HG3	2.01	0.42
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.20	0.42
1:C:279:PRO:HB2	1:C:280:ASP:H	1.75	0.42
1:B:178:PHE:HB2	1:B:212:PHE:CD2	2.55	0.41
1:C:9:ASP:HB3	1:C:11:PHE:CE2	2.55	0.41
1:A:14:GLY:HA2	1:A:52:THR:OG1	2.20	0.41
1:B:49:TYR:CE2	1:B:85:ILE:HD11	2.55	0.41
1:C:208:ARG:HD3	1:C:208:ARG:HH11	1.42	0.41
1:C:161:ALA:O	1:C:165:LEU:HG	2.20	0.41
1:D:20:TRP:CE2	1:D:22:ALA:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.80	0.41
1:A:35:ASP:HA	1:A:36:PRO:HD3	1.93	0.41
1:B:217:GLU:HA	1:B:245:ASP:O	2.21	0.41
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.17	0.41
1:B:152:SER:HB2	4:D:565:HOH:O	2.21	0.41
1:A:164:LEU:HD23	1:A:164:LEU:C	2.41	0.40
1:A:178:PHE:HB2	1:A:212:PHE:CD2	2.56	0.40
1:B:100:LYS:NZ	4:B:402:HOH:O	2.49	0.40
1:B:361:ARG:HA	1:B:365:GLU:OE1	2.21	0.40
1:B:186:GLU:HA	1:B:187:PRO:HA	1.89	0.40
1:C:79:LEU:HA	1:C:79:LEU:HD23	1.96	0.40
1:B:206:LEU:O	1:B:209:PRO:HD3	2.21	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%)	377 (97%)	12 (3%)	1 (0%)	41	50
1	B	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	41	50
1	C	390/393 (99%)	374 (96%)	12 (3%)	4 (1%)	15	17
1	D	390/393 (99%)	376 (96%)	12 (3%)	2 (0%)	29	35
All	All	1560/1572 (99%)	1503 (96%)	49 (3%)	8 (0%)	29	35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	280	ASP
1	A	186	GLU
1	B	186	GLU

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

### 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	305/309 (99%)	296 (97%)	9 (3%)	41	57
1	B	305/309 (99%)	300 (98%)	5 (2%)	62	78
1	C	305/309 (99%)	299 (98%)	6 (2%)	55	72
1	D	305/309 (99%)	297 (97%)	8 (3%)	46	63
All	All	1220/1236 (99%)	1192 (98%)	28 (2%)	50	67

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

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Mol	Chain	Res	Type
1	C	80	ASP
1	C	158	TYR
1	C	203	VAL
1	C	313	ARG
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

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	185	ASN
1	A	204	GLN
1	A	238	HIS
1	B	238	HIS
1	C	41	HIS
1	C	185	ASN
1	C	222	GLN
1	C	238	HIS
1	D	41	HIS
1	D	185	ASN
1	D	204	GLN
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 monosaccharides 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	XLS	D	397	3	8,9,9	2.43	1 (12%)	10,11,11	1.39	1 (10%)
2	XLS	B	397	3	8,9,9	2.42	1 (12%)	10,11,11	2.32	3 (30%)
2	XLS	C	397	3	8,9,9	2.43	1 (12%)	10,11,11	1.67	1 (10%)
2	XLS	A	397	3	8,9,9	2.42	1 (12%)	10,11,11	1.45	1 (10%)

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	XLS	D	397	3	-	0/10/12/12	-
2	XLS	B	397	3	-	2/10/12/12	-
2	XLS	C	397	3	-	0/10/12/12	-
2	XLS	A	397	3	-	1/10/12/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	397	XLS	O1-C1	6.83	1.47	1.19
2	A	397	XLS	O1-C1	6.78	1.47	1.19
2	D	397	XLS	O1-C1	6.71	1.46	1.19
2	B	397	XLS	O1-C1	6.69	1.46	1.19

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	XLS	O4-C4-C3	5.51	122.50	109.10
2	C	397	XLS	O4-C4-C3	4.05	118.95	109.10
2	A	397	XLS	O4-C4-C3	3.93	118.67	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	XLS	O2-C2-C3	-2.76	102.90	109.46
2	B	397	XLS	O3-C3-C2	-2.70	104.22	109.17
2	D	397	XLS	O2-C2-C1	-2.38	104.46	110.08

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	397	XLS	O4-C4-C5-O5
2	A	397	XLS	O4-C4-C5-O5
2	B	397	XLS	O3-C3-C4-C5

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.