



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:20 PM GMT

PDB ID : 4XIA  
Title : STRUCTURES OF D-XYLOSE ISOMERASE FROM ARTHROBACTER STRAIN B3728 CONTAINING THE INHIBITORS XYLITOL AND D-SORBITOL AT 2.5 ANGSTROMS AND 2.3 ANGSTROMS RESOLUTION, RESPECTIVELY  
Authors : Henrick, K.; Collyer, C.A.; Blow, D.M.  
Deposited on : 1989-07-05  
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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

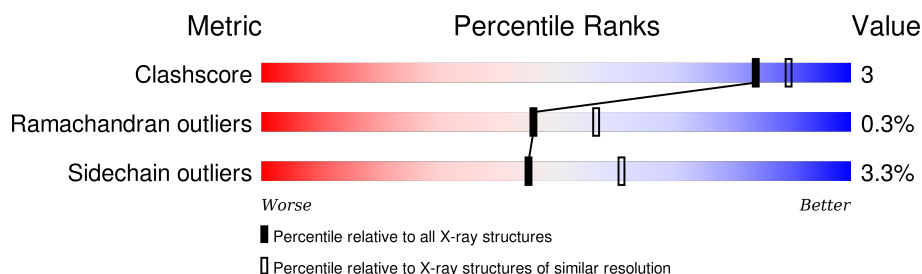
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (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. 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	 75% 22% ..
1	B	393	 78% 18% ..

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6618 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.

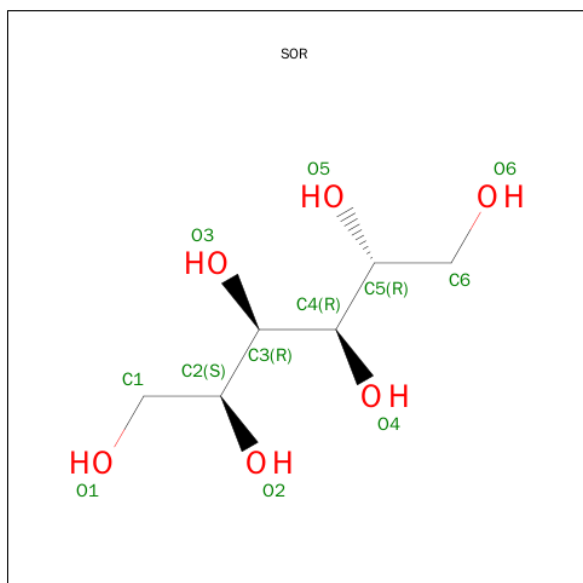
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3027	1919	520	579	9			
1	B	393	Total	C	N	O	S	0	0	0
			3027	1919	520	579	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ALA	LYS	CONFLICT	UNP P12070
A	64	ALA	GLU	CONFLICT	UNP P12070
A	79	ALA	LYS	CONFLICT	UNP P12070
B	31	ALA	LYS	CONFLICT	UNP P12070
B	64	ALA	GLU	CONFLICT	UNP P12070
B	79	ALA	LYS	CONFLICT	UNP P12070

- Molecule 2 is D-SORBITOL (three-letter code: SOR) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- 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		

- Molecule 4 is water.

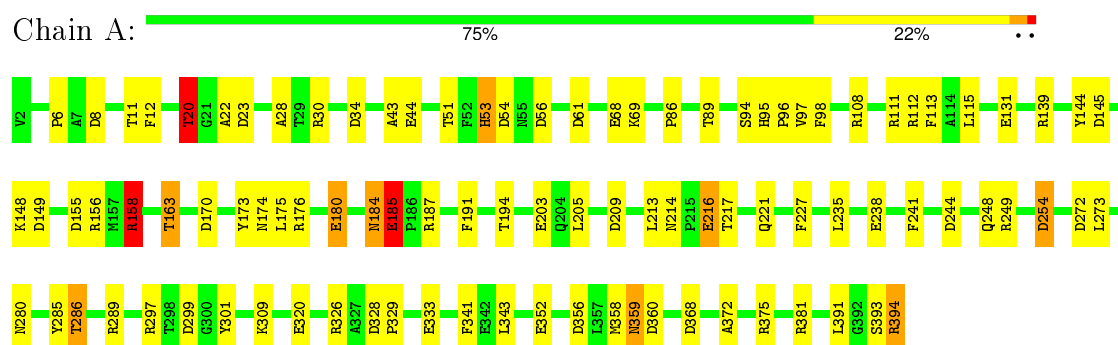
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	268	Total	O	0	0
			268	268		
4	B	270	Total	O	0	0
			270	270		

### 3 Residue-property plots

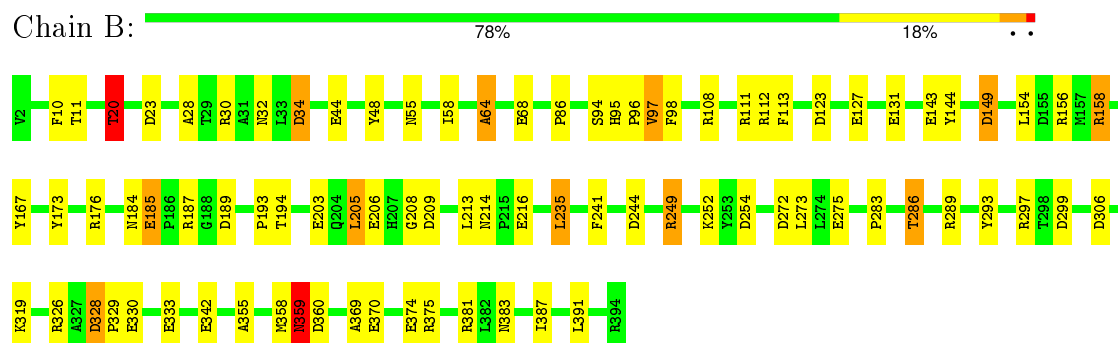
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.80 Å   105.80 Å   153.40 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.147 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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, SOR

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	1.11	2/3101 (0.1%)	2.11	108/4204 (2.6%)
1	B	1.13	2/3101 (0.1%)	2.07	92/4204 (2.2%)
All	All	1.12	4/6202 (0.1%)	2.09	200/8408 (2.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	158	ARG	CD-NE	-7.61	1.33	1.46
1	A	158	ARG	CD-NE	-7.25	1.34	1.46
1	A	158	ARG	CG-CD	-5.40	1.38	1.51
1	B	216	GLU	CD-OE2	5.07	1.31	1.25

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ARG	CD-NE-CZ	31.65	167.91	123.60
1	B	158	ARG	NE-CZ-NH2	-21.33	109.64	120.30
1	A	289	ARG	CD-NE-CZ	18.33	149.27	123.60
1	B	108	ARG	NE-CZ-NH1	17.64	129.12	120.30
1	A	112	ARG	NE-CZ-NH2	17.44	129.02	120.30
1	B	381	ARG	NE-CZ-NH2	-16.07	112.27	120.30
1	A	375	ARG	NE-CZ-NH2	-15.68	112.46	120.30
1	B	30	ARG	NE-CZ-NH2	15.22	127.91	120.30
1	B	187	ARG	NE-CZ-NH1	14.88	127.74	120.30
1	B	158	ARG	NE-CZ-NH1	14.74	127.67	120.30
1	B	358	MET	C-N-CA	14.57	158.14	121.70
1	B	187	ARG	NE-CZ-NH2	-14.16	113.22	120.30
1	A	111	ARG	NE-CZ-NH1	13.72	127.16	120.30
1	B	111	ARG	NE-CZ-NH1	13.23	126.92	120.30
1	B	289	ARG	CD-NE-CZ	12.83	141.56	123.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	ARG	NE-CZ-NH2	12.75	126.67	120.30
1	B	108	ARG	NE-CZ-NH2	-12.38	114.11	120.30
1	B	158	ARG	CD-NE-CZ	12.33	140.86	123.60
1	A	368	ASP	CB-CG-OD1	11.85	128.96	118.30
1	A	23	ASP	CB-CG-OD1	11.81	128.93	118.30
1	A	176	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	A	108	ARG	NE-CZ-NH1	11.60	126.10	120.30
1	B	299	ASP	CB-CG-OD1	11.50	128.65	118.30
1	A	254	ASP	CB-CG-OD2	-11.37	108.07	118.30
1	B	381	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	A	301	TYR	CB-CG-CD1	-11.11	114.33	121.00
1	B	375	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	A	241	PHE	CB-CG-CD1	10.80	128.36	120.80
1	A	375	ARG	NE-CZ-NH1	10.79	125.70	120.30
1	A	139	ARG	NE-CZ-NH1	10.73	125.67	120.30
1	B	112	ARG	CD-NE-CZ	10.45	138.23	123.60
1	A	187	ARG	NE-CZ-NH1	10.33	125.46	120.30
1	A	299	ASP	CB-CG-OD1	10.21	127.49	118.30
1	B	244	ASP	CB-CG-OD1	10.14	127.43	118.30
1	B	123	ASP	CB-CG-OD1	9.94	127.25	118.30
1	B	289	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	A	320	GLU	OE1-CD-OE2	-9.76	111.59	123.30
1	A	158	ARG	NE-CZ-NH2	-9.67	115.47	120.30
1	B	326	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	B	20	THR	N-CA-CB	-9.20	92.82	110.30
1	A	145	ASP	CB-CG-OD1	9.09	126.48	118.30
1	B	249	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	A	156	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	A	170	ASP	CB-CG-OD1	8.95	126.36	118.30
1	A	241	PHE	CB-CG-CD2	-8.95	114.53	120.80
1	B	306	ASP	CB-CG-OD1	8.92	126.33	118.30
1	B	158	ARG	CG-CD-NE	8.85	130.38	111.80
1	A	358	MET	C-N-CA	8.70	143.45	121.70
1	B	254	ASP	CB-CG-OD2	-8.53	110.62	118.30
1	A	112	ARG	CD-NE-CZ	8.41	135.37	123.60
1	A	320	GLU	CA-CB-CG	8.37	131.82	113.40
1	A	68	GLU	OE1-CD-OE2	8.36	133.34	123.30
1	A	297	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	B	108	ARG	CD-NE-CZ	8.19	135.06	123.60
1	A	216	GLU	OE1-CD-OE2	8.14	133.07	123.30
1	B	30	ARG	NE-CZ-NH1	-8.11	116.25	120.30
1	A	320	GLU	CG-CD-OE1	8.08	134.45	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	TYR	CB-CG-CD2	-8.05	116.17	121.00
1	B	156	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	A	238	GLU	OE1-CD-OE2	7.91	132.79	123.30
1	B	359	ASN	CA-CB-CG	7.84	130.64	113.40
1	A	185	GLU	CG-CD-OE1	7.75	133.80	118.30
1	A	113	PHE	CB-CG-CD1	-7.71	115.40	120.80
1	A	30	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	B	144	TYR	CB-CG-CD2	-7.59	116.45	121.00
1	A	194	THR	CA-CB-CG2	7.49	122.89	112.40
1	A	112	ARG	NH1-CZ-NH2	-7.42	111.24	119.40
1	A	209	ASP	CB-CG-OD2	7.41	124.97	118.30
1	B	23	ASP	CB-CA-C	7.39	125.18	110.40
1	B	241	PHE	CB-CG-CD2	-7.38	115.63	120.80
1	B	143	GLU	OE1-CD-OE2	-7.32	114.51	123.30
1	A	187	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	158	ARG	CG-CD-NE	7.31	127.15	111.80
1	B	113	PHE	CB-CG-CD1	-7.24	115.73	120.80
1	A	289	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	B	127	GLU	CA-CB-CG	7.19	129.21	113.40
1	B	23	ASP	CB-CG-OD2	7.18	124.77	118.30
1	A	360	ASP	CB-CG-OD1	7.16	124.74	118.30
1	A	6	PRO	C-N-CA	7.15	139.57	121.70
1	B	44	GLU	CG-CD-OE2	-7.14	104.02	118.30
1	A	352	GLU	OE1-CD-OE2	-7.13	114.74	123.30
1	B	189	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	B	328	ASP	CB-CG-OD1	7.07	124.66	118.30
1	B	286	THR	N-CA-CB	-7.00	97.01	110.30
1	B	360	ASP	CB-CG-OD1	6.98	124.59	118.30
1	A	20	THR	N-CA-CB	-6.97	97.05	110.30
1	B	209	ASP	CB-CG-OD1	6.97	124.58	118.30
1	A	131	GLU	CB-CG-CD	6.97	133.02	114.20
1	A	372	ALA	O-C-N	-6.79	111.83	122.70
1	A	297	ARG	CD-NE-CZ	6.79	133.10	123.60
1	B	213	LEU	CA-CB-CG	6.76	130.85	115.30
1	B	203	GLU	CG-CD-OE1	6.67	131.63	118.30
1	B	254	ASP	CB-CG-OD1	6.61	124.25	118.30
1	B	111	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	111	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	34	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	173	TYR	CB-CG-CD2	6.48	124.89	121.00
1	A	381	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	6	PRO	O-C-N	-6.40	112.47	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	149	ASP	CB-CG-OD1	6.37	124.03	118.30
1	B	154	LEU	CB-CA-C	6.35	122.27	110.20
1	A	155	ASP	CB-CG-OD1	-6.35	112.59	118.30
1	B	144	TYR	CB-CG-CD1	6.33	124.80	121.00
1	B	149	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	51	THR	CA-CB-CG2	6.32	121.25	112.40
1	B	34	ASP	CB-CG-OD1	6.31	123.98	118.30
1	B	97	VAL	CA-CB-CG1	6.31	120.36	110.90
1	A	43	ALA	CB-CA-C	6.29	119.54	110.10
1	B	359	ASN	N-CA-CB	-6.25	99.35	110.60
1	A	333	GLU	CA-CB-CG	6.24	127.12	113.40
1	A	56	ASP	N-CA-CB	6.23	121.82	110.60
1	B	131	GLU	OE1-CD-OE2	-6.22	115.83	123.30
1	A	8	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	139	ARG	NH1-CZ-NH2	-6.20	112.58	119.40
1	A	297	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	20	THR	CA-CB-CG2	6.17	121.04	112.40
1	A	352	GLU	CG-CD-OE1	6.16	130.63	118.30
1	A	144	TYR	CB-CG-CD1	6.14	124.68	121.00
1	B	375	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	173	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	A	44	GLU	CA-CB-CG	6.07	126.74	113.40
1	B	64	ALA	N-CA-CB	6.06	118.59	110.10
1	A	203	GLU	OE1-CD-OE2	-6.04	116.05	123.30
1	B	374	GLU	OE1-CD-OE2	-6.03	116.07	123.30
1	B	98	PHE	O-C-N	-6.01	113.08	122.70
1	B	176	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	B	10	PHE	CB-CG-CD1	5.94	124.96	120.80
1	B	113	PHE	CB-CG-CD2	5.93	124.95	120.80
1	A	368	ASP	OD1-CG-OD2	-5.88	112.13	123.30
1	A	149	ASP	N-CA-C	-5.84	95.23	111.00
1	A	108	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	48	TYR	N-CA-CB	-5.75	100.25	110.60
1	A	30	ARG	CD-NE-CZ	5.74	131.63	123.60
1	A	44	GLU	N-CA-CB	5.72	120.90	110.60
1	B	20	THR	CB-CA-C	5.71	127.03	111.60
1	B	149	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	369	ALA	CB-CA-C	5.71	118.66	110.10
1	B	123	ASP	OD1-CG-OD2	-5.70	112.48	123.30
1	A	176	ARG	NH1-CZ-NH2	-5.68	113.15	119.40
1	B	149	ASP	N-CA-C	-5.65	95.74	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	112	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	A	286	THR	CA-CB-OG1	-5.62	97.19	109.00
1	B	374	GLU	CG-CD-OE1	5.62	129.54	118.30
1	A	53	HIS	CB-CA-C	-5.57	99.26	110.40
1	A	249	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	156	ARG	CA-CB-CG	5.52	125.55	113.40
1	A	163	THR	CA-CB-CG2	5.52	120.13	112.40
1	A	326	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	B	330	GLU	CA-CB-CG	5.51	125.52	113.40
1	A	96	PRO	O-C-N	-5.46	113.96	122.70
1	B	167	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	A	131	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	A	22	ALA	N-CA-CB	-5.46	102.46	110.10
1	B	289	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	149	ASP	N-CA-CB	5.44	120.39	110.60
1	A	393	SER	C-N-CA	5.44	135.30	121.70
1	A	352	GLU	N-CA-C	-5.43	96.34	111.00
1	A	56	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	214	ASN	CB-CG-ND2	5.40	129.65	116.70
1	B	272	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	358	MET	CG-SD-CE	5.38	108.81	100.20
1	B	342	GLU	CG-CD-OE2	-5.37	107.56	118.30
1	B	328	ASP	OD1-CG-OD2	-5.37	113.10	123.30
1	B	194	THR	CA-CB-CG2	5.36	119.90	112.40
1	A	158	ARG	CB-CG-CD	5.35	125.51	111.60
1	A	320	GLU	CB-CG-CD	5.34	128.63	114.20
1	A	391	LEU	C-N-CA	5.32	133.47	122.30
1	A	98	PHE	CB-CG-CD1	-5.32	117.08	120.80
1	A	155	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	174	ASN	C-N-CA	5.30	134.94	121.70
1	A	175	LEU	CB-CA-C	-5.30	100.14	110.20
1	A	254	ASP	CB-CG-OD1	5.29	123.07	118.30
1	A	185	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	A	272	ASP	CB-CG-OD1	5.27	123.05	118.30
1	B	203	GLU	C-N-CA	5.24	134.80	121.70
1	B	32	ASN	CA-CB-CG	-5.24	101.87	113.40
1	B	173	TYR	CB-CG-CD2	5.23	124.14	121.00
1	B	391	LEU	C-N-CA	5.23	133.29	122.30
1	B	249	ARG	CA-C-N	5.23	126.66	116.20
1	A	180	GLU	CG-CD-OE1	5.22	128.74	118.30
1	A	356	ASP	CB-CG-OD1	5.22	123.00	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	TYR	CB-CG-CD1	5.19	124.11	121.00
1	B	193	PRO	O-C-N	-5.12	114.50	122.70
1	A	54	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	241	PHE	CB-CG-CD1	5.11	124.38	120.80
1	A	180	GLU	CG-CD-OE2	-5.10	108.10	118.30
1	B	359	ASN	CB-CA-C	5.09	120.58	110.40
1	B	205	LEU	O-C-N	5.09	130.84	122.70
1	A	285	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	B	333	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	A	343	LEU	C-N-CA	5.05	132.91	122.30
1	B	293	TYR	CG-CD2-CE2	-5.05	117.26	121.30
1	B	96	PRO	O-C-N	-5.04	114.63	122.70
1	A	359	ASN	CA-CB-CG	5.03	124.47	113.40
1	A	12	PHE	CB-CG-CD1	-5.02	117.28	120.80
1	A	301	TYR	CB-CG-CD2	5.02	124.01	121.00
1	A	394	ARG	N-CA-C	-5.01	97.47	111.00
1	B	206	GLU	OE1-CD-OE2	5.01	129.31	123.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3027	0	2890	18	0
1	B	3027	0	2890	17	0
2	A	12	0	12	0	0
2	B	12	0	11	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	268	0	0	0	0
4	B	270	0	0	2	0
All	All	6618	0	5803	35	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (35) 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:95:HIS:HD2	1:A:97:VAL:H	1.30	0.77
1:B:95:HIS:HD2	1:B:97:VAL:H	1.36	0.74
1:A:158:ARG:HG3	1:A:205:LEU:HD23	1.73	0.70
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.72	0.70
1:A:235:LEU:HD12	1:A:273:LEU:HD21	1.77	0.66
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.87	0.56
1:A:95:HIS:CD2	1:A:97:VAL:H	2.19	0.56
1:B:20:THR:HG23	1:B:28:ALA:CB	2.37	0.54
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.91	0.52
1:B:158:ARG:HG3	1:B:205:LEU:HD23	1.91	0.52
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.74	0.51
1:A:20:THR:HG23	1:A:28:ALA:CB	2.40	0.51
1:B:208:GLY:HA3	4:B:602:HOH:O	2.12	0.49
1:A:184:ASN:HD22	1:A:185:GLU:HB2	1.78	0.49
1:B:249:ARG:O	1:B:252:LYS:HE3	2.15	0.47
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.81	0.46
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.97	0.45
1:A:216:GLU:HB2	1:A:244:ASP:HB2	1.97	0.45
1:B:328:ASP:HA	1:B:329:PRO:HD3	1.74	0.45
1:B:158:ARG:HD2	4:B:489:HOH:O	2.16	0.45
1:B:355:ALA:O	1:B:359:ASN:HB3	2.16	0.45
1:B:64:ALA:O	1:B:68:GLU:HG2	2.16	0.45
1:B:235:LEU:HD22	1:B:283:PRO:HB2	1.99	0.45
1:B:235:LEU:HD12	1:B:273:LEU:HD21	1.99	0.44
1:A:328:ASP:HA	1:A:329:PRO:HD3	1.85	0.44
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.51	0.44
1:A:20:THR:HG23	1:A:28:ALA:HB1	1.98	0.43
1:B:383:ASN:O	1:B:387:ILE:HG12	2.19	0.43
1:A:180:GLU:HG3	1:A:214:ASN:O	2.20	0.42
1:B:55:ASN:HA	1:B:58:ILE:O	2.19	0.42
1:A:217:THR:HA	1:A:227:PHE:CD2	2.56	0.41
1:B:95:HIS:CD2	1:B:97:VAL:H	2.26	0.41
1:A:115:LEU:HD21	1:A:163:THR:HG21	2.03	0.41
1:A:309:LYS:HB2	1:A:309:LYS:HE2	1.86	0.41
1:A:280:ASN:OD1	1:A:341:PHE:HA	2.22	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	391/393 (100%)	377 (96%)	13 (3%)	1 (0%)	46	57
1	B	391/393 (100%)	379 (97%)	11 (3%)	1 (0%)	46	57
All	All	782/786 (100%)	756 (97%)	24 (3%)	2 (0%)	46	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU
1	B	185	GLU

### 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	305/306 (100%)	295 (97%)	10 (3%)	45	61
1	B	305/306 (100%)	295 (97%)	10 (3%)	45	61
All	All	610/612 (100%)	590 (97%)	20 (3%)	45	61

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	69	LYS
1	A	94	SER
1	A	158	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	184	ASN
1	A	213	LEU
1	A	254	ASP
1	A	286	THR
1	A	359	ASN
1	A	394	ARG
1	B	20	THR
1	B	34	ASP
1	B	94	SER
1	B	149	ASP
1	B	184	ASN
1	B	185	GLU
1	B	235	LEU
1	B	286	THR
1	B	359	ASN
1	B	370	GLU

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	75	ASN
1	A	95	HIS
1	A	184	ASN
1	A	221	GLN
1	A	384	GLN
1	B	95	HIS
1	B	120	HIS
1	B	184	ASN
1	B	221	GLN
1	B	359	ASN
1	B	384	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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	$\# Z  > 2$
2	SOR	A	400	3	11,11,11	1.81	2 (18%)	14,14,14	2.93	6 (42%)
2	SOR	B	400	3	11,11,11	2.00	2 (18%)	14,14,14	3.51	10 (71%)

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	SOR	A	400	3	-	0/16/16/16	0/0/0/0
2	SOR	B	400	3	-	0/16/16/16	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	SOR	O5-C5	-3.43	1.35	1.43
2	A	400	SOR	C4-C3	3.07	1.59	1.53
2	A	400	SOR	O3-C3	4.38	1.53	1.43
2	B	400	SOR	O3-C3	5.02	1.55	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	SOR	C2-C3-C4	-8.51	98.63	112.47
2	B	400	SOR	C2-C3-C4	-6.26	102.30	112.47
2	B	400	SOR	C5-C4-C3	-5.82	103.00	112.47

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	SOR	C5-C4-C3	-3.83	106.25	112.47
2	B	400	SOR	C6-C5-C4	-3.78	103.62	112.48
2	B	400	SOR	O6-C6-C5	-3.46	103.58	111.10
2	B	400	SOR	O5-C5-C6	-3.25	101.64	109.22
2	B	400	SOR	O4-C4-C5	-3.11	100.92	108.75
2	B	400	SOR	O2-C2-C1	-2.38	103.67	109.22
2	A	400	SOR	O2-C2-C1	-2.31	103.82	109.22
2	A	400	SOR	O3-C3-C4	2.28	114.92	109.45
2	A	400	SOR	O3-C3-C2	2.34	114.66	108.75
2	B	400	SOR	O3-C3-C2	2.73	115.64	108.75
2	A	400	SOR	O2-C2-C3	2.80	116.05	109.02
2	B	400	SOR	O2-C2-C3	3.76	118.47	109.02
2	B	400	SOR	O3-C3-C4	4.32	119.82	109.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.