



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 09:29 PM EST

PDB ID : 1XIM  
Title : ARGININE RESIDUES AS STABILIZING ELEMENTS IN PROTEINS  
Authors : Mrabet, N.T.; Van Denbroek, A.; Van Den Brande, I.; Stanssens, P.; Laroche, Y.; Lambeir, A.-M.; Matthyssens, G.; Jenkins, J.; Chiadmi, M.; Vantilbeurgh, H.; Rey, F.; Janin, J.; Quax, W.J.; Lasters, I.; Demaeyer, M.; Wodak, S.J.  
Deposited on : 1991-05-29  
Resolution : 2.20 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (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) : 2.36

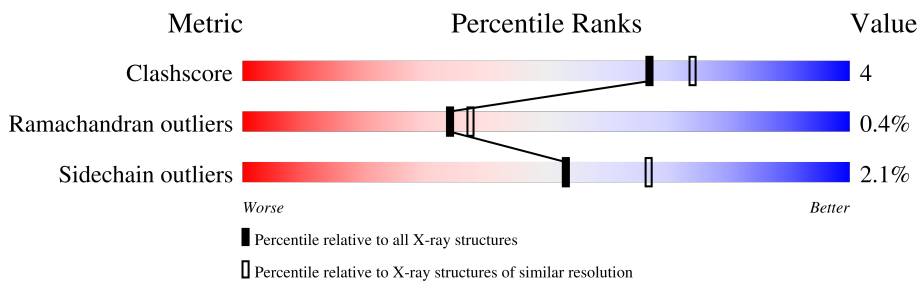
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 [i](#)

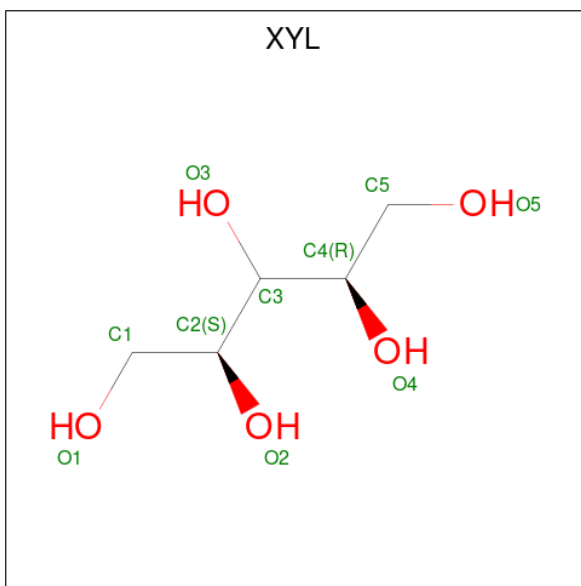
There are 4 unique types of molecules in this entry. The entry contains 13141 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	392	Total 3053	C 1939	N 532	O 578	S 4	0	0	0
1	B	392	Total 3053	C 1939	N 532	O 578	S 4	0	0	0
1	C	392	Total 3053	C 1939	N 532	O 578	S 4	0	0	0
1	D	392	Total 3053	C 1939	N 532	O 578	S 4	0	0	0

- Molecule 2 is Xylitol (three-letter code: XYL) (formula: C<sub>5</sub>H<sub>12</sub>O<sub>5</sub>).



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

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Co 2 2	0	0
3	B	2	Total Co 2 2	0	0
3	C	2	Total Co 2 2	0	0
3	D	2	Total Co 2 2	0	0

- Molecule 4 is water.

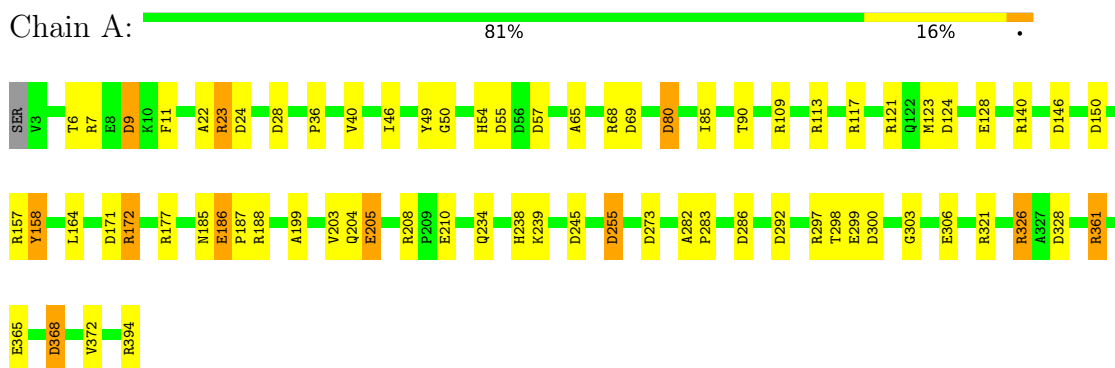
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	225	Total O 225 225	0	0
4	B	212	Total O 212 212	0	0
4	C	233	Total O 233 233	0	0
4	D	211	Total O 211 211	0	0

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

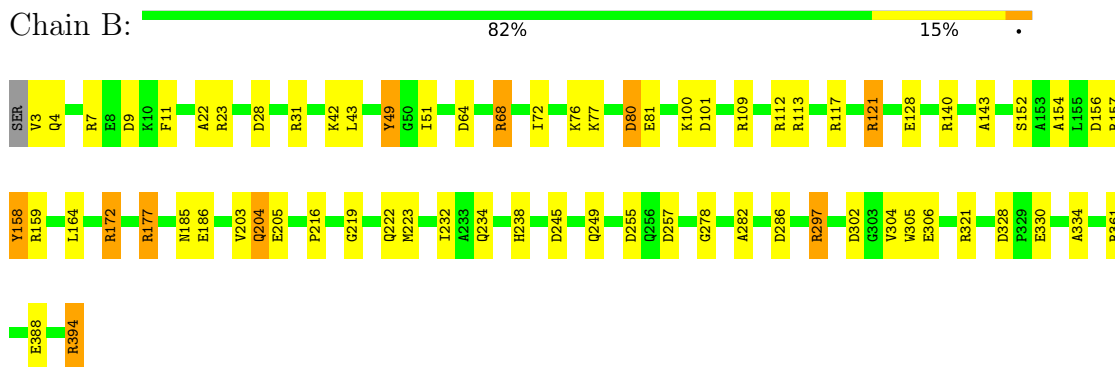
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

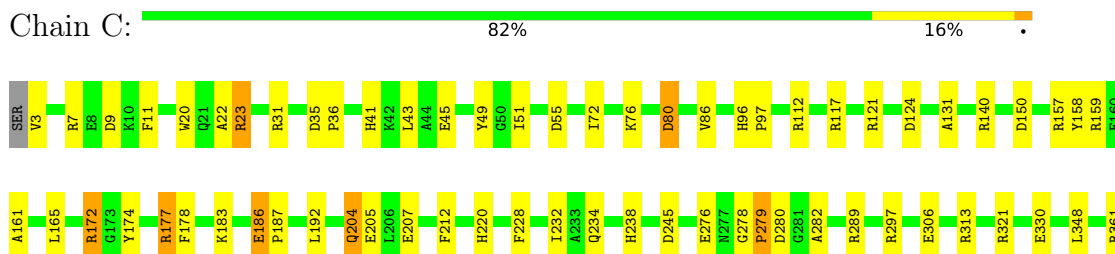
- Molecule 1: D-XYLOSE ISOMERASE



- Molecule 1: D-XYLOSE ISOMERASE



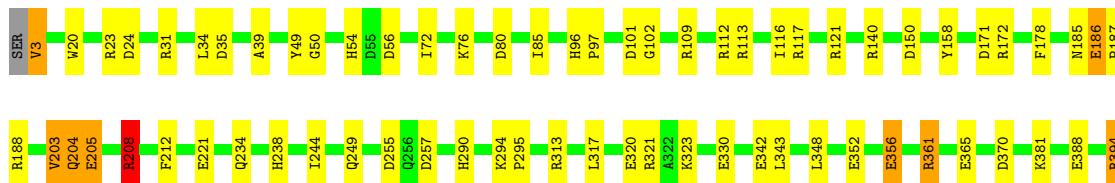
- Molecule 1: D-XYLOSE ISOMERASE





- Molecule 1: D-XYLOSE ISOMERASE

Chain D: 82% 15%



## 4 Data and refinement statistics

Xtrriage (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) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	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.	Xtrriage
Total number of atoms	13141	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	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: XYL, CO

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	0.79	0/3125	1.67	54/4233 (1.3%)
1	B	0.79	0/3125	1.67	49/4233 (1.2%)
1	C	0.79	0/3125	1.64	44/4233 (1.0%)
1	D	0.81	0/3125	1.65	48/4233 (1.1%)
All	All	0.80	0/12500	1.66	195/16932 (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	2
1	B	0	2
1	C	0	2
1	D	0	1
All	All	0	7

There are no bond length outliers.

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	ARG	NE-CZ-NH2	-19.06	110.77	120.30
1	C	172	ARG	NE-CZ-NH2	-18.80	110.90	120.30
1	B	177	ARG	NE-CZ-NH2	-18.59	111.00	120.30
1	B	172	ARG	NE-CZ-NH1	18.52	129.56	120.30
1	C	172	ARG	NE-CZ-NH1	18.41	129.50	120.30
1	D	208	ARG	NE-CZ-NH1	17.55	129.08	120.30
1	D	255	ASP	CB-CG-OD1	17.46	134.02	118.30
1	D	117	ARG	NE-CZ-NH1	16.61	128.60	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	177	ARG	NE-CZ-NH1	15.83	128.22	120.30
1	B	117	ARG	NE-CZ-NH1	15.77	128.19	120.30
1	B	394	ARG	NE-CZ-NH2	-15.66	112.47	120.30
1	A	326	ARG	NE-CZ-NH1	15.44	128.02	120.30
1	A	23	ARG	NE-CZ-NH1	14.51	127.56	120.30
1	A	172	ARG	NE-CZ-NH1	13.41	127.01	120.30
1	D	109	ARG	NE-CZ-NH1	13.20	126.90	120.30
1	C	157	ARG	NE-CZ-NH1	13.15	126.87	120.30
1	D	121	ARG	NE-CZ-NH2	-13.09	113.76	120.30
1	C	177	ARG	NE-CZ-NH2	-12.76	113.92	120.30
1	C	117	ARG	NE-CZ-NH1	12.55	126.58	120.30
1	B	177	ARG	NE-CZ-NH1	12.35	126.47	120.30
1	C	31	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	A	121	ARG	NE-CZ-NH2	-11.75	114.42	120.30
1	A	23	ARG	NE-CZ-NH2	-11.69	114.45	120.30
1	D	150	ASP	CB-CG-OD1	11.69	128.82	118.30
1	D	109	ARG	NE-CZ-NH2	-11.45	114.57	120.30
1	A	394	ARG	NE-CZ-NH1	-11.21	114.70	120.30
1	D	208	ARG	NE-CZ-NH2	-11.07	114.77	120.30
1	C	159	ARG	NE-CZ-NH1	-10.97	114.81	120.30
1	B	117	ARG	NE-CZ-NH2	-10.71	114.95	120.30
1	D	188	ARG	NE-CZ-NH2	10.66	125.63	120.30
1	A	157	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	A	328	ASP	CB-CG-OD2	10.57	127.81	118.30
1	A	326	ARG	NE-CZ-NH2	-10.45	115.07	120.30
1	A	117	ARG	NE-CZ-NH1	10.37	125.49	120.30
1	D	112	ARG	NE-CZ-NH1	10.29	125.45	120.30
1	B	157	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	A	321	ARG	NE-CZ-NH1	10.09	125.35	120.30
1	B	330	GLU	OE1-CD-OE2	10.07	135.38	123.30
1	B	321	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	B	113	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	B	109	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	A	80	ASP	CB-CG-OD1	-9.86	109.43	118.30
1	B	68	ARG	NE-CZ-NH1	-9.70	115.45	120.30
1	A	150	ASP	CB-CG-OD1	9.70	127.03	118.30
1	D	394	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	D	35	ASP	CB-CG-OD1	9.55	126.89	118.30
1	C	245	ASP	CB-CG-OD1	9.47	126.83	118.30
1	C	80	ASP	CB-CG-OD1	-9.40	109.84	118.30
1	C	117	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	A	205	GLU	OE1-CD-OE2	-9.37	112.06	123.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ASP	CB-CG-OD1	9.37	126.73	118.30
1	A	273	ASP	CB-CG-OD1	9.31	126.68	118.30
1	B	302	ASP	CB-CG-OD1	9.28	126.65	118.30
1	A	188	ARG	CD-NE-CZ	9.22	136.51	123.60
1	D	117	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	B	158	TYR	CB-CG-CD2	8.97	126.38	121.00
1	D	313	ARG	NE-CZ-NH2	8.97	124.78	120.30
1	D	255	ASP	CB-CG-OD2	-8.91	110.28	118.30
1	A	146	ASP	CB-CG-OD1	8.82	126.24	118.30
1	B	255	ASP	CB-CG-OD2	-8.78	110.39	118.30
1	A	394	ARG	NH1-CZ-NH2	8.75	129.02	119.40
1	C	23	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	B	140	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	A	172	ARG	NE-CZ-NH2	-8.41	116.10	120.30
1	A	171	ASP	CB-CG-OD1	8.12	125.61	118.30
1	C	140	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	C	321	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	A	394	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	D	208	ARG	CG-CD-NE	8.06	128.74	111.80
1	A	117	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	B	302	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	A	300	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	55	ASP	CB-CG-OD1	7.69	125.22	118.30
1	C	174	TYR	CB-CG-CD2	-7.69	116.38	121.00
1	A	158	TYR	CB-CG-CD2	7.64	125.59	121.00
1	A	68	ARG	NE-CZ-NH2	7.59	124.10	120.30
1	A	121	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	159	ARG	NE-CZ-NH2	7.45	124.02	120.30
1	C	394	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	C	321	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	80	ASP	CA-CB-CG	-7.40	97.11	113.40
1	D	361	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	C	361	ARG	NE-CZ-NH2	7.35	123.97	120.30
1	B	394	ARG	N-CA-CB	7.31	123.76	110.60
1	D	171	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	D	31	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	394	ARG	CA-CB-CG	7.18	129.21	113.40
1	A	255	ASP	CB-CG-OD1	7.04	124.64	118.30
1	B	121	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	C	276	GLU	OE1-CD-OE2	-7.01	114.89	123.30
1	D	330	GLU	OE1-CD-OE2	6.97	131.66	123.30
1	D	113	ARG	NE-CZ-NH1	6.95	123.77	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	GLU	CG-CD-OE2	6.94	132.18	118.30
1	C	150	ASP	CB-CG-OD1	6.93	124.54	118.30
1	C	31	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	D	150	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	B	80	ASP	CB-CG-OD1	-6.82	112.16	118.30
1	A	245	ASP	CB-CG-OD1	6.82	124.44	118.30
1	D	342	GLU	CG-CD-OE2	6.77	131.84	118.30
1	B	112	ARG	NE-CZ-NH2	6.77	123.68	120.30
1	D	257	ASP	CB-CG-OD1	6.76	124.39	118.30
1	D	35	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	A	7	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	D	101	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	109	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	C	174	TYR	CB-CG-CD1	6.65	124.99	121.00
1	B	121	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	255	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	D	112	ARG	CD-NE-CZ	6.62	132.87	123.60
1	C	313	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	361	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	D	370	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	101	ASP	CB-CG-OD2	6.48	124.13	118.30
1	D	56	ASP	CB-CG-OD2	6.44	124.10	118.30
1	B	328	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	55	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	B	112	ARG	NE-CZ-NH1	-6.29	117.16	120.30
1	A	113	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	D	121	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	C	276	GLU	CG-CD-OE2	6.18	130.67	118.30
1	D	205	GLU	OE1-CD-OE2	-6.12	115.96	123.30
1	C	172	ARG	CD-NE-CZ	-6.10	115.06	123.60
1	B	31	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	D	172	ARG	CD-NE-CZ	6.06	132.09	123.60
1	B	255	ASP	CB-CG-OD1	5.99	123.69	118.30
1	D	361	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	B	286	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	9	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	C	150	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	146	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	D	221	GLU	CG-CD-OE1	5.85	130.00	118.30
1	A	140	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	330	GLU	CG-CD-OE2	-5.83	106.64	118.30
1	D	205	GLU	CG-CD-OE2	5.83	129.95	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	23	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	C	55	ASP	CB-CG-OD1	5.76	123.48	118.30
1	D	320	GLU	CA-CB-CG	5.74	126.04	113.40
1	A	368	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	B	394	ARG	CD-NE-CZ	-5.70	115.62	123.60
1	A	158	TYR	CB-CG-CD1	-5.69	117.58	121.00
1	C	207	GLU	CG-CD-OE1	5.67	129.64	118.30
1	C	45	GLU	CA-CB-CG	5.67	125.87	113.40
1	D	54	HIS	N-CA-CB	5.66	120.79	110.60
1	B	156	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	B	158	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	D	342	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	D	321	ARG	NE-CZ-NH2	5.57	123.09	120.30
1	D	31	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	143	ALA	N-CA-CB	-5.55	102.33	110.10
1	A	123	MET	CG-SD-CE	5.54	109.07	100.20
1	C	330	GLU	OE1-CD-OE2	5.54	129.95	123.30
1	B	257	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	245	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	D	203	VAL	CA-CB-CG1	5.49	119.14	110.90
1	C	306	GLU	CG-CD-OE1	5.49	129.27	118.30
1	B	64	ASP	CB-CG-OD1	-5.48	113.36	118.30
1	C	204	GLN	OE1-CD-NE2	-5.46	109.33	121.90
1	D	204	GLN	OE1-CD-NE2	-5.46	109.34	121.90
1	C	306	GLU	CG-CD-OE2	-5.45	107.41	118.30
1	C	140	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	388	GLU	CG-CD-OE1	-5.42	107.46	118.30
1	C	121	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	B	361	ARG	CD-NE-CZ	-5.40	116.04	123.60
1	A	321	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	112	ARG	CG-CD-NE	5.38	123.09	111.80
1	D	320	GLU	OE1-CD-OE2	-5.36	116.86	123.30
1	C	140	ARG	CD-NE-CZ	5.36	131.10	123.60
1	C	124	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	80	ASP	OD1-CG-OD2	5.32	133.41	123.30
1	B	297	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	292	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	7	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	203	VAL	CB-CA-C	5.29	121.44	111.40
1	B	68	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	199	ALA	CB-CA-C	5.23	117.95	110.10
1	C	207	GLU	CG-CD-OE2	-5.22	107.86	118.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	GLN	OE1-CD-NE2	-5.19	109.96	121.90
1	C	289	ARG	CD-NE-CZ	5.19	130.86	123.60
1	D	388	GLU	CG-CD-OE2	5.17	128.65	118.30
1	D	24	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	57	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	128	GLU	CG-CD-OE1	-5.11	108.09	118.30
1	B	334	ALA	CB-CA-C	5.09	117.73	110.10
1	D	249	GLN	CA-CB-CG	5.08	124.58	113.40
1	A	28	ASP	CB-CG-OD1	-5.05	113.75	118.30
1	B	305	TRP	CA-CB-CG	-5.05	104.11	113.70
1	B	245	ASP	CB-CG-OD1	5.05	122.84	118.30
1	C	361	ARG	NH1-CZ-NH2	-5.04	113.86	119.40
1	B	23	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	C	159	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	B	394	ARG	NH1-CZ-NH2	5.01	124.92	119.40
1	A	24	ASP	CB-CG-OD1	5.01	122.81	118.30
1	D	356	GLU	CG-CD-OE2	5.01	128.32	118.30
1	B	28	ASP	CB-CG-OD2	-5.00	113.80	118.30
1	B	304	VAL	CA-CB-CG2	5.00	118.40	110.90

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	ARG	Sidechain
1	A	23	ARG	Sidechain
1	B	172	ARG	Sidechain
1	B	177	ARG	Sidechain
1	C	172	ARG	Sidechain
1	C	177	ARG	Sidechain
1	D	208	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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	3053	0	2954	24	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3053	0	2954	28	0
1	C	3053	0	2954	24	0
1	D	3053	0	2954	27	0
2	A	10	0	11	1	0
2	B	10	0	11	1	0
2	C	10	0	11	1	0
2	D	10	0	11	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	225	0	0	2	0
4	B	212	0	0	3	0
4	C	233	0	0	2	0
4	D	211	0	0	4	0
All	All	13141	0	11860	94	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 (94) 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:B:204:GLN:OE1	1:D:204:GLN:OE1	1.54	1.21
1:A:204:GLN:OE1	1:C:204:GLN:OE1	1.58	1.17
2:C:397:XYL:H12	4:C:610:HOH:O	1.52	1.08
2:B:397:XYL:H12	4:B:589:HOH:O	1.60	1.00
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.22	0.86
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.23	0.82
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.25	0.81
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.26	0.80
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.62	0.80
1:A:204:GLN:HG2	4:A:553:HOH:O	1.84	0.76
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.73	0.71
2:D:397:XYL:H12	4:D:598:HOH:O	1.92	0.70
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.80	0.63
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.81	0.63
2:A:397:XYL:H12	4:A:592:HOH:O	1.99	0.61
1:B:3:VAL:HG12	1:B:4:GLN:H	1.66	0.60
1:D:3:VAL:HG23	4:D:593:HOH:O	2.04	0.57
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.87	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:PRO:O	1:A:40:VAL:HG23	2.06	0.56
1:A:65:ALA:O	1:A:69:ASP:HB2	2.06	0.56
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.87	0.55
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.91	0.53
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.91	0.53
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.44	0.53
1:D:72:ILE:O	1:D:76:LYS:HG3	2.09	0.51
1:A:298:THR:HA	1:B:100:LYS:HD2	1.92	0.51
1:A:208:ARG:NH1	1:A:210:GLU:OE2	2.44	0.50
1:D:34:LEU:HD21	1:D:39:ALA:HB2	1.94	0.50
1:C:183:LYS:HG3	1:C:220:HIS:CG	2.47	0.49
1:C:43:LEU:HD12	1:C:51:ILE:HD12	1.93	0.49
1:B:164:LEU:C	1:B:164:LEU:HD23	2.32	0.49
1:D:102:GLY:HA2	1:D:140:ARG:HB2	1.94	0.49
1:B:152:SER:HB2	4:D:564:HOH:O	2.13	0.49
1:D:361:ARG:HB3	1:D:365:GLU:HB2	1.94	0.49
1:B:77:LYS:O	1:B:80:ASP:HB2	2.13	0.48
1:A:6:THR:O	1:A:9:ASP:HB2	2.14	0.48
1:B:278:GLY:CA	1:B:282:ALA:O	2.63	0.47
1:B:278:GLY:HA3	1:B:282:ALA:O	2.14	0.47
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.96	0.47
1:B:43:LEU:HD12	1:B:51:ILE:HD12	1.97	0.47
1:C:41:HIS:HE1	4:C:521:HOH:O	1.99	0.46
1:A:299:GLU:HB3	1:A:303:GLY:HA3	1.96	0.46
1:C:23:ARG:CZ	1:D:23:ARG:HD2	2.46	0.46
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.51	0.46
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.14	0.45
1:A:186:GLU:HA	1:A:187:PRO:HA	1.75	0.45
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.51	0.45
1:B:121:ARG:HD3	4:B:440:HOH:O	2.16	0.45
1:D:20:TRP:CE3	1:D:294:LYS:HB3	2.52	0.44
1:D:34:LEU:CD2	1:D:39:ALA:HB2	2.47	0.44
1:C:72:ILE:O	1:C:76:LYS:HG3	2.18	0.44
1:D:178:PHE:HB2	1:D:212:PHE:CD2	2.53	0.44
1:D:394:ARG:NH1	4:D:603:HOH:O	2.34	0.44
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.99	0.44
1:C:178:PHE:HB2	1:C:212:PHE:CD2	2.52	0.43
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.79	0.43
1:B:68:ARG:HH11	1:B:68:ARG:HG2	1.84	0.43
1:B:216:PRO:HG2	1:B:232:ILE:HD11	2.01	0.42
1:C:161:ALA:O	1:C:165:LEU:HG	2.19	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:GLU:HA	1:C:187:PRO:HA	1.90	0.42
1:C:228:PHE:CZ	1:C:232:ILE:HD11	2.54	0.42
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.96	0.42
1:B:22:ALA:HB1	1:B:297:ARG:HG3	2.00	0.42
1:A:186:GLU:OE1	1:A:255:ASP:HB3	2.19	0.42
1:B:219:GLY:O	1:B:223:MET:HG3	2.20	0.42
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.85	0.42
1:C:86:VAL:O	1:C:131:ALA:HA	2.20	0.42
1:D:244:ILE:O	1:D:290:HIS:HB3	2.20	0.42
1:C:278:GLY:HA3	1:C:282:ALA:O	2.20	0.42
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.19	0.41
1:B:76:LYS:NZ	1:B:128:GLU:OE2	2.44	0.41
1:A:368:ASP:O	1:A:372:VAL:HG23	2.21	0.41
1:C:192:LEU:HA	1:C:192:LEU:HD23	1.85	0.41
1:D:116:ILE:HD13	1:D:116:ILE:HG21	1.84	0.41
1:B:100:LYS:NZ	4:B:401:HOH:O	2.51	0.41
1:A:164:LEU:HD12	1:C:348:LEU:HD11	2.02	0.41
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.21	0.41
1:B:9:ASP:HB3	1:B:11:PHE:CE2	2.56	0.41
1:D:317:LEU:HD23	1:D:317:LEU:HA	1.87	0.41
1:B:394:ARG:HH11	1:B:394:ARG:HD3	1.69	0.41
1:A:238:HIS:O	1:A:239:LYS:HB2	2.21	0.41
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.94	0.41
1:A:50:GLY:HA2	1:A:85:ILE:O	2.21	0.40
1:B:72:ILE:O	1:B:76:LYS:HG3	2.21	0.40
1:C:9:ASP:HB3	1:C:11:PHE:CE2	2.57	0.40
1:D:186:GLU:HA	1:D:187:PRO:HA	1.80	0.40
1:C:20:TRP:CE2	1:C:22:ALA:HA	2.56	0.40
1:A:326:ARG:HA	1:A:326:ARG:HD3	1.91	0.40
1:B:42:LYS:HD3	1:B:42:LYS:HA	1.99	0.40
1:D:294:LYS:HA	1:D:295:PRO:HD3	1.90	0.40
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.90	0.40
1:A:306:GLU:HG2	1:D:381:LYS:HB2	2.03	0.40
1:B:7:ARG:HG2	1:B:49:TYR:HB2	2.03	0.40
1:D:50:GLY:HA2	1:D:85:ILE:O	2.21	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	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	41	46
1	B	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	41	46
1	C	390/393 (99%)	375 (96%)	11 (3%)	4 (1%)	15	14
1	D	390/393 (99%)	375 (96%)	14 (4%)	1 (0%)	41	46
All	All	1560/1572 (99%)	1502 (96%)	51 (3%)	7 (0%)	34	37

All (7) 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	C	364	PHE
1	D	186	GLU

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/310 (99%)	298 (97%)	8 (3%)	46	58
1	B	306/310 (99%)	301 (98%)	5 (2%)	62	76
1	C	306/310 (99%)	301 (98%)	5 (2%)	62	76

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	306/310 (99%)	298 (97%)	8 (3%)	46 58
All	All	1224/1240 (99%)	1198 (98%)	26 (2%)	53 67

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

Mol	Chain	Res	Type
1	A	46	ILE
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	286	ASP
1	B	49	TYR
1	B	81	GLU
1	B	158	TYR
1	B	185	ASN
1	B	203	VAL
1	C	3	VAL
1	C	49	TYR
1	C	80	ASP
1	C	158	TYR
1	C	279	PRO
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	185	ASN
1	C	238	HIS
1	D	185	ASN
1	D	238	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 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	C	397	3	9,9,9	0.50	0	11,11,11	1.93	4 (36%)
2	XYL	D	397	3	9,9,9	0.51	0	11,11,11	1.53	1 (9%)
2	XYL	A	397	3	9,9,9	0.54	0	11,11,11	1.29	2 (18%)
2	XYL	B	397	3	9,9,9	0.52	0	11,11,11	2.03	3 (27%)

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	397	XYL	O4-C4-C3	4.87	120.94	109.10
2	C	397	XYL	C1-C2-C3	3.64	120.31	112.41
2	B	397	XYL	C1-C2-C3	3.33	119.63	112.41
2	D	397	XYL	O2-C2-C1	-3.30	101.41	109.14
2	C	397	XYL	O4-C4-C3	2.77	115.83	109.10
2	B	397	XYL	O2-C2-C1	-2.64	102.96	109.14
2	A	397	XYL	O4-C4-C3	2.51	115.20	109.10
2	C	397	XYL	O5-C5-C4	-2.34	105.98	111.07
2	A	397	XYL	O2-C2-C1	-2.21	103.95	109.14
2	C	397	XYL	C5-C4-C3	-2.14	107.78	112.41

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	397	XYL	O4-C4-C5-O5
2	A	397	XYL	O4-C4-C5-O5

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.