



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:57 AM UTC

PDB ID : 5XIA / pdb_00005xia
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
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Deposited on : 1989-07-05
Resolution : 2.50 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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

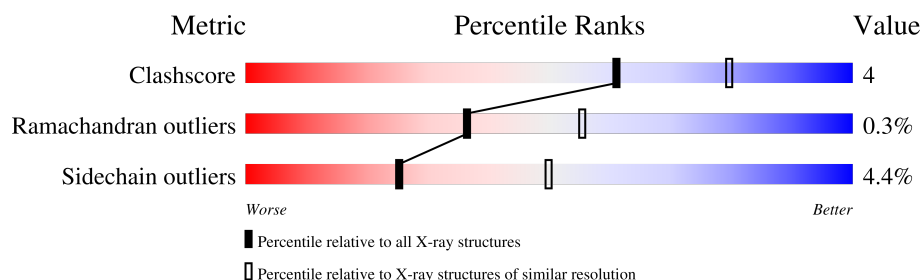
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 ≥ 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	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6651 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.

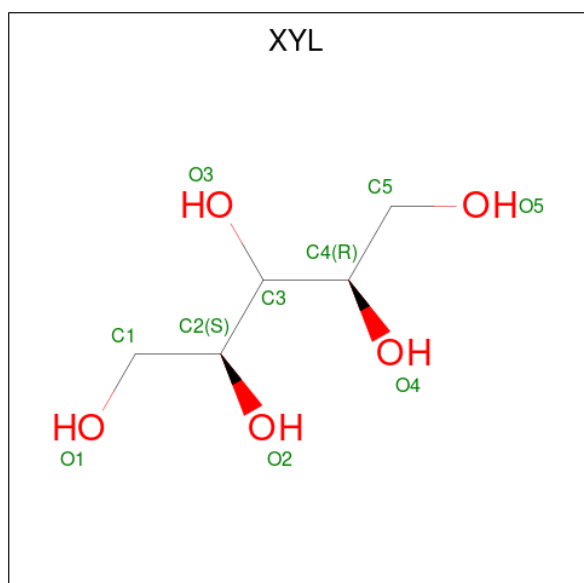
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

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 Xylitol (CCD ID: XYL) (formula: C₅H₁₂O₅).



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		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is water.

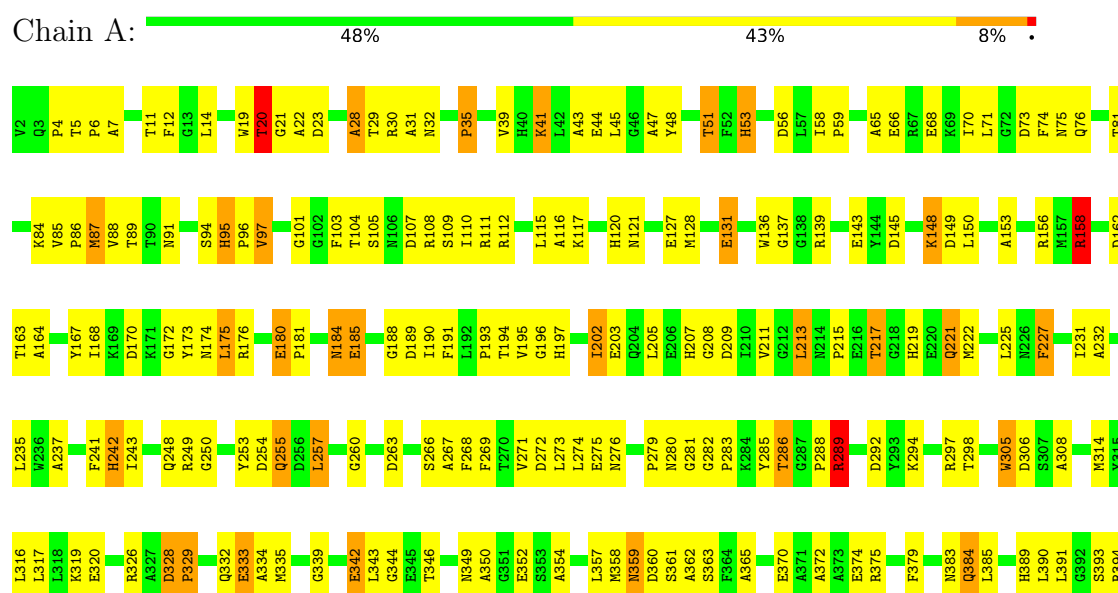
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	283	Total	O	0	0
			283	283		
4	B	292	Total	O	0	0
			292	292		

3 Residue-property plots

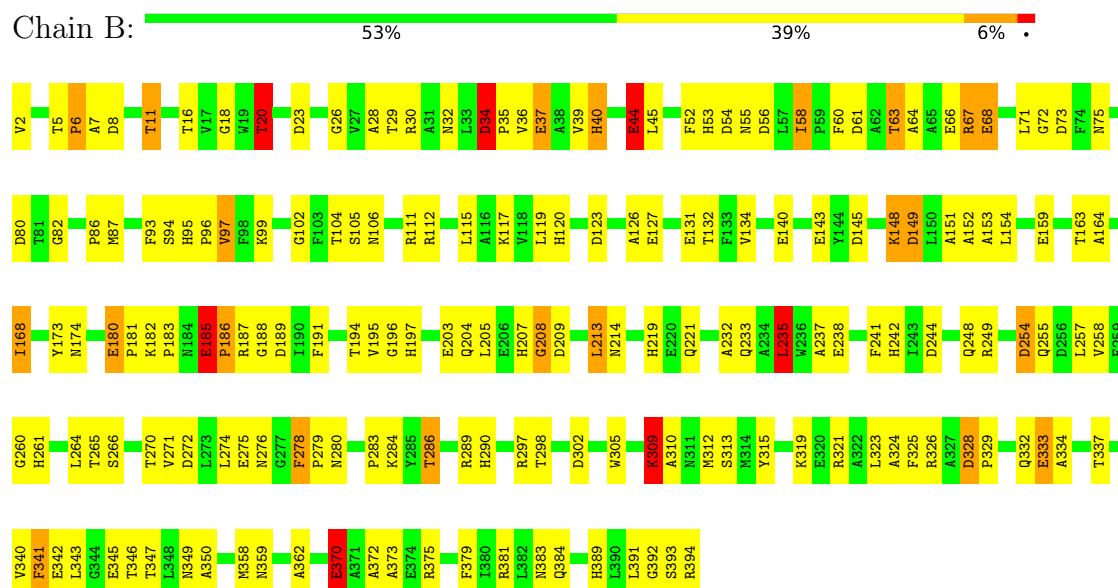
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.90 Å 105.90 Å 153.60 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.135 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6651	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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, XYL

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	1.55	15/3101 (0.5%)	2.82	331/4204 (7.9%)
1	B	1.55	20/3101 (0.6%)	2.67	268/4204 (6.4%)
All	All	1.55	35/6202 (0.6%)	2.74	599/8408 (7.1%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	ARG	CD-NE	-9.09	1.33	1.46
1	B	233	GLN	C-O	8.54	1.34	1.24
1	B	340	VAL	C-O	6.54	1.31	1.24
1	A	281	GLY	N-CA	6.50	1.52	1.45
1	B	265	THR	C-O	6.37	1.31	1.24
1	A	339	GLY	C-O	6.10	1.32	1.23
1	A	286	THR	CA-CB	6.08	1.63	1.54
1	B	373	ALA	C-O	6.07	1.31	1.24
1	B	286	THR	CA-CB	6.03	1.62	1.53
1	B	221	GLN	C-O	5.96	1.31	1.24
1	B	104	THR	CB-OG1	5.87	1.53	1.43
1	A	289	ARG	NE-CZ	-5.69	1.26	1.33
1	B	305	TRP	C-O	5.68	1.31	1.24
1	A	267	ALA	C-O	5.67	1.30	1.24
1	B	276	ASN	C-O	5.62	1.31	1.24
1	A	385	LEU	C-O	5.57	1.30	1.24
1	B	266	SER	C-O	5.57	1.30	1.24
1	B	242	HIS	C-O	5.52	1.30	1.23
1	A	282	GLY	N-CA	5.49	1.52	1.44
1	A	190	ILE	N-CA	5.48	1.53	1.46
1	A	105	SER	C-O	5.47	1.30	1.23
1	A	53	HIS	C-O	5.38	1.30	1.23
1	B	152	ALA	C-O	5.38	1.30	1.24
1	A	110	ILE	CA-CB	5.36	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	392	GLY	N-CA	-5.35	1.38	1.45
1	B	315	TYR	C-O	5.32	1.30	1.24
1	B	99	LYS	C-O	5.31	1.30	1.24
1	B	254	ASP	CA-CB	-5.16	1.46	1.53
1	A	104	THR	CA-CB	5.14	1.60	1.53
1	B	275	GLU	C-O	5.11	1.30	1.24
1	B	105	SER	C-O	5.09	1.29	1.23
1	A	306	ASP	C-O	5.08	1.29	1.24
1	B	16	THR	C-O	5.07	1.29	1.24
1	A	20	THR	CA-C	-5.06	1.45	1.52
1	B	20	THR	C-O	5.00	1.30	1.24

All (599) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	ARG	CD-NE-CZ	38.28	178.00	124.40
1	B	238	GLU	CA-CB-CG	13.66	141.41	114.10
1	B	68	GLU	CB-CG-CD	12.96	134.63	112.60
1	A	394	ARG	CD-NE-CZ	12.77	142.27	124.40
1	A	112	ARG	NE-CZ-NH2	12.50	130.45	119.20
1	A	112	ARG	CD-NE-CZ	12.39	141.75	124.40
1	B	174	ASN	OD1-CG-ND2	-12.04	110.56	122.60
1	A	359	ASN	CA-CB-CG	11.66	124.26	112.60
1	B	343	LEU	CA-C-N	11.29	134.56	120.22
1	B	343	LEU	C-N-CA	11.29	134.56	120.22
1	B	37	GLU	CB-CG-CD	10.96	131.24	112.60
1	A	107	ASP	CA-CB-CG	10.89	123.49	112.60
1	A	32	ASN	CA-CB-CG	-10.75	101.85	112.60
1	B	379	PHE	CA-CB-CG	10.69	124.49	113.80
1	A	6	PRO	CA-C-N	10.69	138.57	120.72
1	A	6	PRO	C-N-CA	10.69	138.57	120.72
1	A	249	ARG	NE-CZ-NH1	10.66	132.16	121.50
1	A	208	GLY	CA-C-N	10.60	134.48	120.28
1	A	208	GLY	C-N-CA	10.60	134.48	120.28
1	B	6	PRO	CA-C-N	10.60	135.54	120.28
1	B	6	PRO	C-N-CA	10.60	135.54	120.28
1	B	131	GLU	CB-CG-CD	10.57	130.58	112.60
1	A	131	GLU	CB-CG-CD	10.36	130.22	112.60
1	A	328	ASP	CA-C-O	10.36	129.75	119.49
1	A	243	ILE	CA-C-O	-10.36	111.23	120.96
1	A	393	SER	CA-C-N	10.26	140.17	121.70
1	A	393	SER	C-N-CA	10.26	140.17	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	GLU	CB-CG-CD	10.07	129.72	112.60
1	A	358	MET	CA-C-N	10.05	134.57	120.29
1	A	358	MET	C-N-CA	10.05	134.57	120.29
1	B	241	PHE	CA-CB-CG	9.92	123.72	113.80
1	B	381	ARG	CD-NE-CZ	9.80	138.12	124.40
1	B	2	VAL	CA-C-N	9.61	135.44	122.56
1	B	2	VAL	C-N-CA	9.61	135.44	122.56
1	B	391	LEU	CA-C-N	9.53	138.67	120.66
1	B	391	LEU	C-N-CA	9.53	138.67	120.66
1	A	75	ASN	OD1-CG-ND2	-9.41	113.19	122.60
1	B	30	ARG	NE-CZ-NH2	9.36	127.63	119.20
1	A	143	GLU	CA-C-O	9.35	131.09	119.78
1	B	342	GLU	CB-CG-CD	9.34	128.48	112.60
1	B	20	THR	N-CA-CB	-9.24	94.89	110.41
1	A	320	GLU	CB-CG-CD	9.17	128.20	112.60
1	B	99	LYS	CA-C-O	-9.17	109.74	120.10
1	A	286	THR	CA-CB-OG1	-9.13	95.90	109.60
1	B	58	ILE	O-C-N	9.04	129.52	121.12
1	B	93	PHE	CA-C-O	-8.98	108.23	118.47
1	A	127	GLU	CA-CB-CG	8.98	132.06	114.10
1	B	145	ASP	CA-C-O	-8.87	109.77	119.97
1	B	324	ALA	CA-C-N	8.78	132.24	120.65
1	B	324	ALA	C-N-CA	8.78	132.24	120.65
1	A	372	ALA	O-C-N	-8.74	112.85	122.12
1	A	235	LEU	O-C-N	-8.74	113.06	122.07
1	B	328	ASP	CA-C-O	8.70	128.03	119.51
1	A	394	ARG	NE-CZ-NH2	-8.69	111.38	119.20
1	A	349	ASN	CA-CB-CG	8.63	121.23	112.60
1	B	53	HIS	CA-CB-CG	8.61	122.41	113.80
1	A	43	ALA	O-C-N	-8.60	112.80	122.09
1	B	286	THR	N-CA-CB	-8.59	97.42	110.73
1	B	163	THR	CA-C-O	-8.56	111.83	120.82
1	B	334	ALA	CA-C-N	8.54	131.73	120.28
1	B	334	ALA	C-N-CA	8.54	131.73	120.28
1	B	358	MET	CA-C-N	8.53	138.07	121.18
1	B	358	MET	C-N-CA	8.53	138.07	121.18
1	B	106	ASN	CA-C-N	8.53	133.52	121.24
1	B	106	ASN	C-N-CA	8.53	133.52	121.24
1	B	298	THR	CA-C-N	8.51	135.32	122.65
1	B	298	THR	C-N-CA	8.51	135.32	122.65
1	A	44	GLU	N-CA-CB	8.50	122.62	110.12
1	A	286	THR	N-CA-CB	-8.45	98.23	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ALA	CA-C-O	-8.42	111.89	121.15
1	A	19	TRP	CA-C-O	8.41	130.33	120.58
1	A	174	ASN	CA-CB-CG	-8.36	104.24	112.60
1	A	43	ALA	CB-CA-C	8.35	124.09	110.90
1	B	56	ASP	CA-CB-CG	8.33	120.93	112.60
1	B	20	THR	CB-CA-C	8.31	126.48	109.95
1	A	156	ARG	CD-NE-CZ	8.30	136.01	124.40
1	A	149	ASP	N-CA-CB	8.28	122.69	110.35
1	A	110	ILE	O-C-N	-8.25	113.82	121.91
1	A	101	GLY	O-C-N	8.23	131.17	123.35
1	A	111	ARG	CA-C-N	8.21	131.11	120.44
1	A	111	ARG	C-N-CA	8.21	131.11	120.44
1	B	61	ASP	CA-CB-CG	-8.18	104.42	112.60
1	B	96	PRO	O-C-N	-8.16	112.30	122.17
1	B	319	LYS	CB-CG-CD	8.15	130.04	111.30
1	B	244	ASP	CA-CB-CG	8.13	120.73	112.60
1	A	222	MET	CA-C-N	8.06	134.99	122.49
1	A	222	MET	C-N-CA	8.06	134.99	122.49
1	B	112	ARG	CD-NE-CZ	8.05	135.68	124.40
1	A	297	ARG	CA-C-N	8.05	134.36	120.68
1	A	297	ARG	C-N-CA	8.05	134.36	120.68
1	A	235	LEU	CA-C-N	8.04	131.39	120.38
1	A	235	LEU	C-N-CA	8.04	131.39	120.38
1	B	188	GLY	CA-C-N	8.04	134.10	122.77
1	B	188	GLY	C-N-CA	8.04	134.10	122.77
1	A	271	VAL	CA-C-N	8.02	131.37	120.54
1	A	271	VAL	C-N-CA	8.02	131.37	120.54
1	A	103	PHE	CA-CB-CG	8.00	121.80	113.80
1	A	389	HIS	CA-C-O	-7.98	112.48	120.70
1	B	164	ALA	CA-C-N	7.98	131.62	120.29
1	B	164	ALA	C-N-CA	7.98	131.62	120.29
1	B	214	ASN	CB-CG-ND2	7.97	128.36	116.40
1	B	248	GLN	OE1-CD-NE2	-7.91	114.69	122.60
1	B	67	ARG	CG-CD-NE	7.89	129.37	112.00
1	B	6	PRO	O-C-N	-7.87	112.02	122.64
1	B	207	HIS	CA-C-N	7.86	130.03	120.13
1	B	207	HIS	C-N-CA	7.86	130.03	120.13
1	B	94	SER	N-CA-C	7.82	121.31	111.69
1	B	313	SER	CA-C-N	7.81	131.65	120.79
1	B	313	SER	C-N-CA	7.81	131.65	120.79
1	B	207	HIS	CA-CB-CG	-7.81	105.99	113.80
1	A	180	GLU	CA-C-O	7.80	126.96	119.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	HIS	CA-C-O	-7.80	112.63	120.82
1	A	354	ALA	CA-C-N	7.78	131.61	120.79
1	A	354	ALA	C-N-CA	7.78	131.61	120.79
1	A	235	LEU	CB-CA-C	7.78	123.09	110.88
1	B	290	HIS	CA-C-O	7.78	128.91	120.43
1	A	362	ALA	CA-C-N	7.77	132.12	120.31
1	A	362	ALA	C-N-CA	7.77	132.12	120.31
1	B	32	ASN	CA-CB-CG	-7.77	104.83	112.60
1	A	215	PRO	CA-C-O	-7.76	112.21	121.67
1	A	273	LEU	CA-C-O	-7.69	112.78	120.70
1	A	391	LEU	CA-C-N	7.64	136.39	121.41
1	A	391	LEU	C-N-CA	7.64	136.39	121.41
1	B	23	ASP	CB-CA-C	7.63	125.21	110.17
1	B	375	ARG	NE-CZ-NH2	-7.62	112.34	119.20
1	A	174	ASN	N-CA-CB	7.60	123.15	110.53
1	B	195	VAL	CA-C-O	-7.59	113.37	121.27
1	A	221	GLN	CA-C-N	7.57	133.36	120.72
1	A	221	GLN	C-N-CA	7.57	133.36	120.72
1	A	289	ARG	CG-CD-NE	7.57	128.66	112.00
1	A	320	GLU	CA-CB-CG	7.57	129.24	114.10
1	A	271	VAL	O-C-N	-7.55	114.51	121.91
1	A	335	MET	CA-C-O	7.52	128.52	120.55
1	A	389	HIS	N-CA-CB	7.50	120.95	110.07
1	A	150	LEU	CA-C-O	-7.49	112.61	120.55
1	A	175	LEU	O-C-N	7.48	132.16	123.41
1	B	309	LYS	CA-C-N	7.47	130.63	120.54
1	B	309	LYS	C-N-CA	7.47	130.63	120.54
1	B	332	GLN	CA-C-O	-7.41	112.69	120.55
1	A	329	PRO	CA-C-N	7.41	130.54	120.54
1	A	329	PRO	C-N-CA	7.41	130.54	120.54
1	B	120	HIS	CA-C-N	7.36	131.50	120.31
1	B	120	HIS	C-N-CA	7.36	131.50	120.31
1	A	19	TRP	N-CA-CB	7.32	120.99	109.71
1	A	286	THR	N-CA-C	7.32	123.23	113.72
1	B	71	LEU	CA-C-N	7.32	127.92	119.94
1	B	71	LEU	C-N-CA	7.32	127.92	119.94
1	A	235	LEU	CA-C-O	7.30	128.49	120.82
1	A	208	GLY	O-C-N	-7.30	114.51	122.54
1	A	127	GLU	O-C-N	-7.27	114.42	122.12
1	A	285	TYR	CA-C-N	-7.23	110.76	122.26
1	A	285	TYR	C-N-CA	-7.23	110.76	122.26
1	B	8	ASP	CA-C-N	7.22	132.38	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	ASP	C-N-CA	7.22	132.38	122.19
1	B	289	ARG	CD-NE-CZ	7.20	134.48	124.40
1	A	194	THR	CA-CB-CG2	7.17	122.70	110.50
1	A	21	GLY	N-CA-C	7.16	123.39	114.37
1	B	241	PHE	CA-C-O	-7.16	110.89	119.27
1	A	44	GLU	CA-CB-CG	7.14	128.39	114.10
1	B	323	LEU	N-CA-C	-7.14	103.43	111.14
1	A	163	THR	CA-CB-OG1	-7.13	98.91	109.60
1	A	136	TRP	CA-C-O	-7.12	112.84	120.46
1	A	48	TYR	N-CA-C	-7.11	104.23	113.12
1	A	120	HIS	CA-C-N	7.11	130.52	120.28
1	A	120	HIS	C-N-CA	7.11	130.52	120.28
1	A	209	ASP	CA-C-O	-7.10	113.03	120.55
1	B	117	LYS	CA-C-N	7.10	129.65	120.56
1	B	117	LYS	C-N-CA	7.10	129.65	120.56
1	A	65	ALA	N-CA-C	-7.09	103.24	110.97
1	A	211	VAL	CA-CB-CG2	7.09	122.45	110.40
1	A	32	ASN	OD1-CG-ND2	7.09	129.69	122.60
1	A	289	ARG	NE-CZ-NH2	7.08	125.57	119.20
1	A	346	THR	CA-CB-OG1	-7.08	98.98	109.60
1	B	20	THR	CA-CB-CG2	7.07	122.52	110.50
1	B	381	ARG	NE-CZ-NH2	-7.07	112.84	119.20
1	B	52	PHE	CA-C-O	7.04	128.76	121.23
1	A	158	ARG	CD-NE-CZ	7.00	134.20	124.40
1	A	274	LEU	CA-C-N	6.99	132.38	120.71
1	A	274	LEU	C-N-CA	6.99	132.38	120.71
1	A	394	ARG	NE-CZ-NH1	6.95	128.45	121.50
1	A	172	GLY	CA-C-N	6.95	130.74	120.87
1	A	172	GLY	C-N-CA	6.95	130.74	120.87
1	A	195	VAL	CA-C-N	6.94	127.83	119.99
1	A	195	VAL	C-N-CA	6.94	127.83	119.99
1	B	379	PHE	O-C-N	-6.89	113.80	122.27
1	B	174	ASN	CB-CG-OD1	6.88	134.56	120.80
1	B	346	THR	CA-CB-OG1	-6.87	99.30	109.60
1	B	102	GLY	CA-C-N	6.86	130.39	120.38
1	B	102	GLY	C-N-CA	6.86	130.39	120.38
1	A	305	TRP	CA-C-N	6.83	129.32	120.44
1	A	305	TRP	C-N-CA	6.83	129.32	120.44
1	B	393	SER	N-CA-C	-6.80	104.62	113.12
1	A	149	ASP	N-CA-C	-6.80	96.03	107.99
1	B	159	GLU	CA-C-O	-6.79	113.35	120.55
1	B	302	ASP	CA-C-N	6.79	127.47	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	ASP	C-N-CA	6.79	127.47	120.00
1	A	188	GLY	CA-C-O	-6.76	113.79	120.75
1	B	151	ALA	CA-C-N	6.74	129.31	120.28
1	B	151	ALA	C-N-CA	6.74	129.31	120.28
1	A	19	TRP	CA-C-N	6.74	134.60	122.06
1	A	19	TRP	C-N-CA	6.74	134.60	122.06
1	B	328	ASP	CA-CB-CG	6.74	119.34	112.60
1	A	308	ALA	CA-C-N	6.72	129.58	120.44
1	A	308	ALA	C-N-CA	6.72	129.58	120.44
1	A	168	ILE	CA-C-N	6.69	129.13	120.44
1	A	168	ILE	C-N-CA	6.69	129.13	120.44
1	A	58	ILE	O-C-N	6.68	125.58	121.37
1	B	117	LYS	CG-CD-CE	6.65	126.60	111.30
1	A	148	LYS	CA-C-O	6.64	128.88	121.11
1	B	196	GLY	CA-C-N	6.63	129.06	120.44
1	B	196	GLY	C-N-CA	6.63	129.06	120.44
1	B	127	GLU	CA-CB-CG	6.63	127.36	114.10
1	A	117	LYS	CA-C-O	-6.62	113.48	120.63
1	A	365	ALA	O-C-N	-6.61	115.21	122.09
1	A	66	GLU	O-C-N	-6.61	115.21	122.09
1	B	208	GLY	CA-C-N	6.58	129.76	120.28
1	B	208	GLY	C-N-CA	6.58	129.76	120.28
1	B	298	THR	O-C-N	-6.58	113.37	122.46
1	B	34	ASP	CB-CA-C	6.57	119.74	109.42
1	B	325	PHE	CA-CB-CG	6.57	120.37	113.80
1	B	44	GLU	CG-CD-OE2	-6.57	103.29	118.40
1	A	379	PHE	CA-CB-CG	6.56	120.36	113.80
1	A	383	ASN	O-C-N	-6.55	114.68	122.15
1	A	115	LEU	CB-CA-C	6.54	121.97	110.85
1	A	227	PHE	CA-C-O	-6.52	113.64	120.55
1	B	36	VAL	CA-C-N	6.49	128.88	120.44
1	B	36	VAL	C-N-CA	6.49	128.88	120.44
1	A	360	ASP	CA-C-N	6.49	130.17	120.31
1	A	360	ASP	C-N-CA	6.49	130.17	120.31
1	B	56	ASP	N-CA-CB	6.49	120.33	110.28
1	B	60	PHE	CA-C-N	6.48	134.11	122.06
1	B	60	PHE	C-N-CA	6.48	134.11	122.06
1	A	158	ARG	O-C-N	-6.47	115.26	122.12
1	A	289	ARG	NE-CZ-NH1	-6.47	115.03	121.50
1	A	85	VAL	CA-C-N	6.46	126.04	119.19
1	A	85	VAL	C-N-CA	6.46	126.04	119.19
1	A	266	SER	CA-C-O	-6.46	113.70	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	ASP	CA-CB-CG	6.45	119.05	112.60
1	B	264	LEU	N-CA-C	6.44	117.96	111.07
1	A	14	LEU	O-C-N	-6.42	115.31	122.12
1	A	263	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	20	THR	CA-C-N	-6.42	114.42	123.08
1	A	20	THR	C-N-CA	-6.42	114.42	123.08
1	A	73	ASP	CA-CB-CG	6.42	119.02	112.60
1	B	143	GLU	CA-C-O	6.39	126.63	119.41
1	A	35	PRO	CA-C-N	6.39	128.61	120.56
1	A	35	PRO	C-N-CA	6.39	128.61	120.56
1	B	7	ALA	N-CA-CB	-6.38	100.39	110.22
1	B	290	HIS	CA-CB-CG	6.38	120.18	113.80
1	A	71	LEU	CA-C-N	6.36	127.00	119.94
1	A	71	LEU	C-N-CA	6.36	127.00	119.94
1	A	5	THR	N-CA-C	-6.36	100.37	110.10
1	A	174	ASN	OD1-CG-ND2	6.34	128.94	122.60
1	A	203	GLU	CG-CD-OE1	6.33	132.97	118.40
1	A	87	MET	O-C-N	-6.33	115.93	123.27
1	B	111	ARG	CA-C-N	6.31	128.74	120.28
1	B	111	ARG	C-N-CA	6.31	128.74	120.28
1	A	6	PRO	O-C-N	-6.31	114.12	122.64
1	A	158	ARG	CA-C-N	6.30	129.55	120.79
1	A	158	ARG	C-N-CA	6.30	129.55	120.79
1	A	280	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	A	352	GLU	CA-C-O	-6.30	114.03	120.71
1	B	16	THR	CA-C-O	6.29	127.40	120.80
1	A	20	THR	CA-C-O	-6.28	111.70	119.18
1	B	286	THR	OG1-CB-CG2	6.28	121.85	109.30
1	B	333	GLU	CA-CB-CG	6.28	126.65	114.10
1	A	243	ILE	O-C-N	6.27	129.21	123.19
1	A	70	ILE	CA-C-O	-6.27	114.75	121.27
1	B	362	ALA	CA-C-O	-6.26	112.77	119.97
1	A	354	ALA	CA-C-O	6.26	127.95	121.07
1	A	29	THR	CA-C-O	6.25	125.93	119.05
1	B	149	ASP	N-CA-C	-6.25	97.52	108.20
1	A	203	GLU	CB-CG-CD	6.24	123.20	112.60
1	A	372	ALA	CA-C-N	6.23	133.51	121.18
1	A	372	ALA	C-N-CA	6.23	133.51	121.18
1	B	194	THR	CA-CB-CG2	6.22	121.08	110.50
1	B	271	VAL	CA-C-N	6.22	128.94	120.54
1	B	271	VAL	C-N-CA	6.22	128.94	120.54
1	A	96	PRO	CA-C-N	6.21	129.29	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	PRO	C-N-CA	6.21	129.29	120.53
1	B	34	ASP	CA-C-N	6.21	126.11	119.28
1	B	34	ASP	C-N-CA	6.21	126.11	119.28
1	B	383	ASN	CA-C-O	-6.21	114.30	120.82
1	A	352	GLU	CB-CG-CD	6.21	123.15	112.60
1	A	120	HIS	O-C-N	-6.20	115.55	122.12
1	A	107	ASP	CA-C-O	6.20	127.76	120.69
1	B	384	GLN	OE1-CD-NE2	-6.20	116.40	122.60
1	B	30	ARG	NE-CZ-NH1	-6.19	115.31	121.50
1	B	163	THR	CA-CB-OG1	-6.18	100.34	109.60
1	A	250	GLY	N-CA-C	6.17	120.81	112.17
1	A	276	ASN	CA-C-O	-6.17	112.05	119.27
1	A	333	GLU	CA-C-N	6.16	128.54	120.28
1	A	333	GLU	C-N-CA	6.16	128.54	120.28
1	A	352	GLU	N-CA-C	-6.16	99.67	109.59
1	A	167	TYR	O-C-N	-6.16	115.73	122.07
1	A	51	THR	CA-CB-CG2	6.15	120.96	110.50
1	A	235	LEU	N-CA-CB	-6.15	101.09	110.01
1	A	7	ALA	CA-C-N	6.14	129.64	120.31
1	A	7	ALA	C-N-CA	6.14	129.64	120.31
1	B	221	GLN	OE1-CD-NE2	-6.14	116.46	122.60
1	A	145	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	350	ALA	CB-CA-C	6.13	119.47	109.90
1	A	298	THR	CA-C-N	6.13	131.16	122.09
1	A	298	THR	C-N-CA	6.13	131.16	122.09
1	A	96	PRO	O-C-N	-6.12	114.76	122.17
1	A	357	LEU	CA-C-O	-6.12	113.93	120.42
1	A	332	GLN	CB-CG-CD	6.12	123.00	112.60
1	A	363	SER	N-CA-C	6.11	118.90	111.82
1	A	45	LEU	CA-C-O	-6.10	111.87	119.38
1	A	334	ALA	O-C-N	-6.09	115.66	122.12
1	A	56	ASP	N-CA-CB	6.08	119.16	110.16
1	B	36	VAL	CB-CA-C	6.07	120.60	112.22
1	B	255	GLN	CG-CD-NE2	6.07	125.50	116.40
1	A	116	ALA	CA-C-N	6.07	128.69	120.38
1	A	116	ALA	C-N-CA	6.07	128.69	120.38
1	A	342	GLU	CB-CA-C	-6.06	100.38	110.68
1	A	359	ASN	CB-CA-C	-6.06	100.55	110.85
1	B	11	THR	O-C-N	-6.06	115.32	123.19
1	A	232	ALA	CA-C-O	-6.05	114.00	120.42
1	B	270	THR	N-CA-CB	6.05	118.85	110.07
1	A	232	ALA	N-CA-C	-6.05	104.76	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	ARG	NE-CZ-NH2	-6.04	113.76	119.20
1	A	84	LYS	O-C-N	-6.04	116.20	123.03
1	A	156	ARG	CA-CB-CG	6.04	126.18	114.10
1	B	80	ASP	CA-C-N	6.04	132.90	122.09
1	B	80	ASP	C-N-CA	6.04	132.90	122.09
1	A	158	ARG	CB-CG-CD	6.03	125.17	111.30
1	B	73	ASP	CA-CB-CG	6.02	118.62	112.60
1	B	187	ARG	NE-CZ-NH1	6.02	127.52	121.50
1	A	222	MET	CA-C-O	-6.00	112.00	119.38
1	A	174	ASN	CB-CG-ND2	-5.98	107.43	116.40
1	A	91	ASN	CA-C-O	-5.98	114.70	120.92
1	A	280	ASN	CB-CG-ND2	5.98	125.36	116.40
1	B	16	THR	CA-CB-OG1	-5.97	100.64	109.60
1	A	241	PHE	CB-CG-CD1	5.97	130.84	120.70
1	A	276	ASN	CB-CG-ND2	5.97	125.35	116.40
1	A	53	HIS	N-CA-CB	5.94	120.31	110.52
1	A	320	GLU	CG-CD-OE1	5.93	132.03	118.40
1	B	44	GLU	CG-CD-OE1	5.92	132.03	118.40
1	B	115	LEU	CB-CA-C	5.90	120.15	110.88
1	A	139	ARG	NH1-CZ-NH2	-5.90	111.63	119.30
1	B	214	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	B	394	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	A	189	ASP	CA-C-O	-5.89	113.04	120.28
1	B	272	ASP	CA-C-N	5.89	128.65	120.29
1	B	272	ASP	C-N-CA	5.89	128.65	120.29
1	B	203	GLU	CA-C-N	5.88	131.61	122.49
1	B	203	GLU	C-N-CA	5.88	131.61	122.49
1	B	389	HIS	N-CA-C	-5.88	104.78	111.14
1	B	213	LEU	CA-CB-CG	5.88	136.89	116.30
1	B	7	ALA	CA-C-N	5.88	130.54	120.72
1	B	7	ALA	C-N-CA	5.88	130.54	120.72
1	A	117	LYS	CA-C-N	5.88	128.08	120.56
1	A	117	LYS	C-N-CA	5.88	128.08	120.56
1	A	170	ASP	CA-C-O	-5.88	114.65	120.82
1	B	53	HIS	N-CA-CB	5.88	120.22	110.52
1	A	23	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	375	ARG	CD-NE-CZ	-5.86	116.19	124.40
1	B	56	ASP	N-CA-C	-5.86	105.02	111.82
1	B	310	ALA	O-C-N	-5.86	116.00	122.09
1	A	342	GLU	CA-C-N	5.86	128.72	120.28
1	A	342	GLU	C-N-CA	5.86	128.72	120.28
1	B	321	ARG	CA-CB-CG	-5.85	102.39	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	ALA	CA-C-N	5.85	128.12	120.28
1	B	232	ALA	C-N-CA	5.85	128.12	120.28
1	B	257	LEU	O-C-N	5.85	130.01	122.23
1	A	4	PRO	CA-C-O	5.84	128.32	121.31
1	A	196	GLY	CA-C-N	5.84	128.10	120.28
1	A	196	GLY	C-N-CA	5.84	128.10	120.28
1	B	333	GLU	CA-C-N	5.83	128.10	120.28
1	B	333	GLU	C-N-CA	5.83	128.10	120.28
1	A	255	GLN	N-CA-CB	-5.83	101.52	110.20
1	A	334	ALA	CA-C-N	5.83	128.09	120.28
1	A	334	ALA	C-N-CA	5.83	128.09	120.28
1	A	193	PRO	N-CA-C	5.83	121.20	113.57
1	A	163	THR	CA-CB-CG2	5.82	120.40	110.50
1	A	384	GLN	CG-CD-NE2	5.82	125.14	116.40
1	B	188	GLY	O-C-N	-5.82	116.60	122.19
1	B	189	ASP	CA-C-O	-5.82	114.07	120.24
1	A	208	GLY	CA-C-O	5.81	126.50	119.65
1	A	139	ARG	CD-NE-CZ	5.81	132.53	124.40
1	A	95	HIS	CA-C-N	5.79	126.19	119.47
1	A	95	HIS	C-N-CA	5.79	126.19	119.47
1	A	47	ALA	CA-C-O	5.78	128.57	121.87
1	A	221	GLN	O-C-N	-5.78	114.69	122.43
1	B	174	ASN	CA-C-N	5.78	131.82	122.29
1	B	174	ASN	C-N-CA	5.78	131.82	122.29
1	B	310	ALA	CA-C-N	5.78	128.82	120.79
1	B	310	ALA	C-N-CA	5.78	128.82	120.79
1	B	349	ASN	CB-CG-ND2	5.77	125.06	116.40
1	A	225	LEU	N-CA-CB	-5.77	101.65	110.42
1	A	121	ASN	CA-C-N	5.77	128.36	120.46
1	A	121	ASN	C-N-CA	5.77	128.36	120.46
1	B	208	GLY	N-CA-C	5.76	120.94	113.27
1	B	373	ALA	N-CA-C	5.76	119.78	112.87
1	B	54	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	97	VAL	CA-CB-CG1	5.75	120.17	110.40
1	A	352	GLU	CG-CD-OE1	5.74	131.61	118.40
1	A	317	LEU	CA-C-O	-5.74	114.47	120.55
1	A	286	THR	OG1-CB-CG2	5.74	120.77	109.30
1	B	82	GLY	CA-C-O	-5.70	112.50	119.06
1	B	180	GLU	CA-C-O	5.70	124.98	119.62
1	B	37	GLU	CB-CA-C	5.69	119.82	110.88
1	A	137	GLY	CA-C-N	5.69	130.92	120.79
1	A	137	GLY	C-N-CA	5.69	130.92	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	HIS	CA-C-N	5.69	126.29	119.98
1	B	197	HIS	C-N-CA	5.69	126.29	119.98
1	B	249	ARG	O-C-N	-5.68	115.60	122.65
1	A	297	ARG	O-C-N	-5.67	114.89	122.43
1	A	314	MET	N-CA-CB	5.67	118.43	109.82
1	B	319	LYS	CA-C-N	5.66	127.80	120.44
1	B	319	LYS	C-N-CA	5.66	127.80	120.44
1	B	394	ARG	NH1-CZ-NH2	5.66	126.66	119.30
1	B	328	ASP	CA-C-N	5.64	125.31	119.05
1	B	328	ASP	C-N-CA	5.64	125.31	119.05
1	B	242	HIS	CA-C-O	-5.64	115.40	121.38
1	A	185	GLU	CG-CD-OE1	5.64	131.37	118.40
1	A	202	ILE	CA-C-N	5.63	130.13	120.72
1	A	202	ILE	C-N-CA	5.63	130.13	120.72
1	A	269	PHE	CA-CB-CG	-5.63	108.17	113.80
1	A	81	THR	CA-CB-OG1	-5.62	101.17	109.60
1	A	162	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	381	ARG	NH1-CZ-NH2	5.60	126.58	119.30
1	B	159	GLU	O-C-N	5.58	128.03	122.12
1	B	123	ASP	OD1-CG-OD2	-5.57	109.54	122.90
1	B	278	PHE	CA-C-N	5.56	125.66	119.32
1	B	278	PHE	C-N-CA	5.56	125.66	119.32
1	B	389	HIS	N-CA-CB	5.55	118.12	110.07
1	B	40	HIS	CA-CB-CG	-5.55	108.25	113.80
1	A	84	LYS	CA-C-N	5.54	132.38	122.13
1	A	84	LYS	C-N-CA	5.54	132.38	122.13
1	B	312	MET	O-C-N	-5.54	116.37	122.07
1	A	329	PRO	O-C-N	-5.54	115.59	122.23
1	B	235	LEU	CA-C-N	5.53	127.96	120.38
1	B	235	LEU	C-N-CA	5.53	127.96	120.38
1	A	263	ASP	CA-C-O	-5.53	114.35	120.60
1	B	154	LEU	CB-CA-C	5.53	120.82	110.70
1	B	72	GLY	CA-C-O	-5.53	114.71	120.90
1	A	266	SER	CA-C-N	5.53	127.62	120.44
1	A	266	SER	C-N-CA	5.53	127.62	120.44
1	B	274	LEU	O-C-N	5.52	128.05	122.09
1	B	372	ALA	O-C-N	-5.52	116.27	122.12
1	B	64	ALA	CA-C-N	5.50	128.43	120.79
1	B	64	ALA	C-N-CA	5.50	128.43	120.79
1	A	254	ASP	N-CA-CB	5.49	118.61	109.60
1	B	297	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	B	18	GLY	CA-C-N	5.48	130.21	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	GLY	C-N-CA	5.48	130.21	121.66
1	B	341	PHE	N-CA-C	-5.48	104.95	111.69
1	A	139	ARG	NE-CZ-NH1	5.47	126.97	121.50
1	A	374	GLU	O-C-N	-5.46	114.92	122.46
1	A	31	ALA	CA-C-O	-5.46	115.37	121.81
1	A	297	ARG	N-CA-C	5.46	119.42	112.87
1	A	94	SER	N-CA-C	5.46	118.40	111.69
1	A	112	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	A	333	GLU	CA-CB-CG	5.45	125.00	114.10
1	B	298	THR	CA-C-O	5.45	126.07	119.31
1	B	323	LEU	N-CA-CB	5.45	117.97	110.07
1	A	209	ASP	O-C-N	5.44	127.89	122.12
1	B	119	LEU	O-C-N	-5.44	116.36	122.12
1	B	381	ARG	CA-C-N	5.43	127.87	120.54
1	B	381	ARG	C-N-CA	5.43	127.87	120.54
1	B	123	ASP	CB-CG-OD1	5.43	130.88	118.40
1	A	128	MET	CA-C-N	5.43	129.70	120.91
1	A	128	MET	C-N-CA	5.43	129.70	120.91
1	B	134	VAL	CA-CB-CG1	5.43	119.62	110.40
1	A	344	GLY	CA-C-O	-5.42	113.06	119.45
1	A	164	ALA	CA-C-N	5.42	127.98	120.29
1	A	164	ALA	C-N-CA	5.42	127.98	120.29
1	B	254	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	197	HIS	CB-CG-CD2	-5.39	124.19	131.20
1	A	53	HIS	CB-CA-C	-5.39	100.42	109.48
1	A	352	GLU	CA-CB-CG	5.39	124.88	114.10
1	A	22	ALA	N-CA-CB	-5.39	102.05	109.97
1	A	249	ARG	CD-NE-CZ	5.38	131.93	124.40
1	A	195	VAL	CA-C-O	-5.37	115.68	121.27
1	A	127	GLU	CG-CD-OE2	-5.37	106.05	118.40
1	B	44	GLU	N-CA-CB	5.37	118.48	110.22
1	A	326	ARG	CA-C-N	5.36	129.79	120.68
1	A	326	ARG	C-N-CA	5.36	129.79	120.68
1	B	29	THR	CA-CB-OG1	-5.36	101.56	109.60
1	B	260	GLY	O-C-N	-5.35	116.60	122.65
1	A	190	ILE	CA-C-O	-5.35	114.68	121.48
1	A	217	THR	CA-C-N	5.35	127.01	120.22
1	A	217	THR	C-N-CA	5.35	127.01	120.22
1	A	12	PHE	CA-CB-CG	5.35	119.15	113.80
1	A	184	ASN	CA-C-N	5.34	134.83	121.80
1	A	184	ASN	C-N-CA	5.34	134.83	121.80
1	B	126	ALA	O-C-N	-5.34	116.48	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	GLY	CA-C-N	5.33	132.04	122.38
1	A	260	GLY	C-N-CA	5.33	132.04	122.38
1	B	258	VAL	O-C-N	5.33	128.27	122.57
1	B	26	GLY	N-CA-C	5.32	118.84	110.91
1	A	88	VAL	CA-CB-CG2	5.32	119.45	110.40
1	B	153	ALA	CA-C-N	5.32	129.68	120.58
1	B	153	ALA	C-N-CA	5.32	129.68	120.58
1	A	213	LEU	N-CA-C	5.32	118.38	110.14
1	A	231	ILE	CB-CA-C	5.32	120.87	112.26
1	A	68	GLU	CA-C-O	-5.31	113.86	119.97
1	B	204	GLN	CG-CD-NE2	5.31	124.36	116.40
1	A	188	GLY	N-CA-C	-5.30	106.36	112.73
1	A	281	GLY	CA-C-O	-5.30	117.99	122.29
1	B	44	GLU	CB-CG-CD	-5.30	103.58	112.60
1	A	74	PHE	CA-C-O	-5.30	114.80	120.42
1	A	73	ASP	O-C-N	5.30	127.53	122.07
1	B	383	ASN	CA-CB-CG	-5.30	107.30	112.60
1	B	370	GLU	CA-C-O	-5.29	113.88	119.97
1	A	104	THR	CA-CB-CG2	5.29	119.49	110.50
1	B	347	THR	CA-C-O	-5.29	115.27	120.82
1	A	272	ASP	O-C-N	-5.29	116.59	122.09
1	B	145	ASP	O-C-N	5.29	128.77	122.27
1	B	96	PRO	CA-C-N	5.29	128.82	120.47
1	B	96	PRO	C-N-CA	5.29	128.82	120.47
1	B	284	LYS	CA-CB-CG	5.29	124.67	114.10
1	B	93	PHE	O-C-N	5.28	128.14	121.64
1	A	94	SER	CA-C-O	-5.27	114.39	120.24
1	A	219	HIS	CB-CG-ND1	-5.27	114.79	122.70
1	B	237	ALA	CA-C-N	5.26	129.66	122.34
1	B	237	ALA	O-C-N	-5.26	115.11	122.37
1	B	237	ALA	C-N-CA	5.26	129.66	122.34
1	A	76	GLN	CA-C-N	5.26	127.64	120.54
1	A	76	GLN	C-N-CA	5.26	127.64	120.54
1	A	279	PRO	O-C-N	-5.26	116.19	122.24
1	A	59	PRO	CA-C-N	5.25	127.62	120.54
1	A	59	PRO	C-N-CA	5.25	127.62	120.54
1	B	63	THR	N-CA-C	-5.25	103.76	110.53
1	A	231	ILE	CA-C-N	5.24	127.73	120.29
1	A	231	ILE	C-N-CA	5.24	127.73	120.29
1	A	241	PHE	CB-CG-CD2	-5.24	111.79	120.70
1	B	168	ILE	N-CA-CB	5.23	116.12	110.62
1	A	237	ALA	CA-C-N	5.23	130.16	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ALA	C-N-CA	5.23	130.16	122.63
1	A	276	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	A	108	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	20	THR	CB-CA-C	5.21	119.73	109.72
1	B	342	GLU	CG-CD-OE2	-5.21	106.41	118.40
1	B	205	LEU	O-C-N	5.21	128.90	123.06
1	A	286	THR	CB-CA-C	5.21	118.30	109.55
1	A	283	PRO	CB-CA-C	5.20	117.76	110.95
1	B	219	HIS	N-CA-CB	5.20	117.55	110.01
1	A	242	HIS	ND1-CG-CD2	-5.19	100.91	106.10
1	B	203	GLU	CG-CD-OE1	5.19	130.34	118.40
1	A	305	TRP	CB-CA-C	5.19	120.64	110.67
1	A	316	LEU	CB-CA-C	5.18	119.65	110.85
1	A	84	LYS	CA-C-O	5.17	127.97	121.66
1	B	345	GLU	CB-CG-CD	5.16	121.37	112.60
1	B	140	GLU	CB-CG-CD	5.16	121.37	112.60
1	B	174	ASN	CB-CA-C	5.16	119.89	112.05
1	B	186	PRO	N-CA-C	5.15	125.49	112.10
1	A	173	TYR	CA-C-O	-5.15	115.39	121.16
1	A	390	LEU	CA-C-O	-5.14	115.10	120.55
1	B	337	THR	CA-C-N	5.14	131.36	121.18
1	B	337	THR	C-N-CA	5.14	131.36	121.18
1	A	97	VAL	N-CA-CB	5.14	116.89	110.47
1	A	393	SER	CA-CB-OG	-5.13	100.83	111.10
1	B	384	GLN	CA-C-N	5.13	127.58	120.29
1	B	384	GLN	C-N-CA	5.13	127.58	120.29
1	A	30	ARG	CA-C-O	-5.13	115.31	121.11
1	A	292	ASP	CB-CA-C	5.13	119.30	111.76
1	A	109	SER	CB-CA-C	5.12	119.00	110.90
1	B	221	GLN	CA-C-N	5.12	129.28	120.72
1	B	221	GLN	C-N-CA	5.12	129.28	120.72
1	B	248	GLN	CB-CA-C	5.12	118.51	109.80
1	A	268	PHE	O-C-N	-5.12	116.60	122.08
1	B	2	VAL	CA-C-O	5.12	129.50	120.80
1	A	209	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	347	THR	CA-CB-OG1	-5.11	101.94	109.60
1	A	153	ALA	CA-C-O	-5.11	115.44	120.90
1	B	375	ARG	CB-CA-C	-5.11	102.18	109.84
1	A	343	LEU	CA-C-N	5.07	129.67	120.79
1	A	343	LEU	C-N-CA	5.07	129.67	120.79
1	B	194	THR	CA-CB-OG1	-5.07	102.00	109.60
1	B	120	HIS	O-C-N	-5.07	116.04	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ASP	N-CA-C	-5.06	105.84	111.36
1	A	203	GLU	CA-C-N	5.06	130.88	122.54
1	A	203	GLU	C-N-CA	5.06	130.88	122.54
1	B	159	GLU	CG-CD-OE2	-5.05	106.78	118.40
1	B	359	ASN	CB-CA-C	-5.05	99.87	110.17
1	B	5	THR	CA-C-N	5.04	126.14	119.84
1	B	5	THR	C-N-CA	5.04	126.14	119.84
1	A	207	HIS	CA-C-N	5.04	129.40	120.74
1	A	207	HIS	C-N-CA	5.04	129.40	120.74
1	B	350	ALA	CA-C-O	-5.04	115.47	120.96
1	B	64	ALA	N-CA-CB	5.03	117.52	110.12
1	B	127	GLU	O-C-N	-5.03	116.78	122.12
1	B	148	LYS	N-CA-CB	-5.03	102.79	111.55
1	A	273	LEU	N-CA-C	-5.03	105.70	111.14
1	A	257	LEU	CA-CB-CG	5.03	133.90	116.30
1	A	253	TYR	CA-C-N	5.03	129.50	121.66
1	A	253	TYR	C-N-CA	5.03	129.50	121.66
1	A	176	ARG	N-CA-C	-5.01	101.23	109.40
1	B	332	GLN	CA-C-N	5.01	127.25	120.44
1	B	332	GLN	C-N-CA	5.01	127.25	120.44
1	A	263	ASP	CA-C-N	5.01	127.25	120.44
1	A	263	ASP	C-N-CA	5.01	127.25	120.44
1	A	255	GLN	O-C-N	-5.01	115.72	122.23
1	A	249	ARG	NE-CZ-NH2	-5.00	114.70	119.20
1	B	342	GLU	CA-C-N	5.00	128.60	120.60
1	B	342	GLU	C-N-CA	5.00	128.60	120.60

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	2891	25	0
1	B	3027	0	2891	26	0
2	A	10	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	10	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	283	0	0	3	0
4	B	292	0	0	3	0
All	All	6651	0	5803	50	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 (50) 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:275:GLU:HG3	1:A:319:LYS:HG3	1.67	0.76
1:B:95:HIS:HD2	1:B:97:VAL:H	1.34	0.72
1:B:235:LEU:HD22	1:B:283:PRO:HB2	1.76	0.68
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.64	0.62
1:A:294:LYS:HE2	4:A:641:HOH:O	2.02	0.58
1:A:95:HIS:HD2	1:A:97:VAL:H	1.51	0.57
1:B:45:LEU:HD22	1:B:309:LYS:HD3	1.87	0.57
1:A:51:THR:HG21	1:A:87:MET:HE3	1.90	0.53
1:B:55:ASN:HA	1:B:58:ILE:O	2.08	0.53
1:B:208:GLY:HA3	4:B:599:HOH:O	2.09	0.53
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.91	0.53
1:A:158:ARG:HG3	1:A:205:LEU:HD23	1.91	0.51
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.92	0.51
1:A:20:THR:HG23	1:A:28:ALA:HB1	1.95	0.49
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.49	0.48
1:A:370:GLU:HG2	4:A:644:HOH:O	2.13	0.48
1:A:41:LYS:HG2	1:A:305:TRP:CE2	2.49	0.47
1:B:370:GLU:HG2	4:B:678:HOH:O	2.14	0.47
1:B:328:ASP:HA	1:B:329:PRO:HD3	1.69	0.46
1:B:168:ILE:HG23	1:B:173:TYR:HB2	1.96	0.46
1:B:180:GLU:HA	1:B:181:PRO:HD3	1.81	0.45
1:A:158:ARG:HB3	4:A:465:HOH:O	2.16	0.45
1:B:34:ASP:HA	1:B:35:PRO:HD3	1.77	0.45
1:A:328:ASP:HA	1:A:329:PRO:HD3	1.77	0.45
1:B:35:PRO:O	1:B:39:VAL:HG23	2.17	0.45
1:B:20:THR:HG23	1:B:28:ALA:CB	2.47	0.44
1:A:217:THR:HA	1:A:227:PHE:CD2	2.52	0.44
1:A:255:GLN:HB3	1:A:257:LEU:HG	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:PRO:O	1:A:39:VAL:HG23	2.17	0.44
1:B:45:LEU:HD22	1:B:309:LYS:CD	2.47	0.44
1:A:20:THR:HG23	1:A:28:ALA:CB	2.48	0.44
1:B:11:THR:HG21	1:B:86:PRO:HG2	2.00	0.44
1:A:242:HIS:CD2	1:A:288:PRO:HG2	2.54	0.43
1:B:75:ASN:ND2	4:B:665:HOH:O	2.51	0.43
1:A:202:ILE:O	1:A:205:LEU:HB2	2.18	0.43
1:B:148:LYS:HG3	1:B:191:PHE:HZ	1.83	0.43
1:B:280:ASN:OD1	1:B:341:PHE:HA	2.19	0.43
1:B:63:THR:HG23	1:B:66:GLU:OE1	2.20	0.42
1:B:278:PHE:HA	1:B:279:PRO:HD3	1.92	0.42
1:B:185:GLU:HA	1:B:186:PRO:HA	1.84	0.42
1:A:95:HIS:CD2	1:A:97:VAL:H	2.34	0.42
1:A:384:GLN:NE2	1:B:261:HIS:NE2	2.67	0.42
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.85	0.41
1:B:40:HIS:O	1:B:44:GLU:HG3	2.21	0.41
1:A:289:ARG:N	1:A:289:ARG:HD2	2.35	0.41
1:B:182:LYS:HA	1:B:183:PRO:HD3	1.88	0.41
1:A:131:GLU:O	1:A:175:LEU:HA	2.21	0.41
1:B:95:HIS:CD2	1:B:97:VAL:H	2.25	0.40
1:A:180:GLU:HA	1:A:181:PRO:HD3	1.82	0.40
1:B:87:MET:HA	1:B:132:THR: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	391/393 (100%)	377 (96%)	13 (3%)	1 (0%)	36	55
1	B	391/393 (100%)	375 (96%)	15 (4%)	1 (0%)	36	55
All	All	782/786 (100%)	752 (96%)	28 (4%)	2 (0%)	36	55

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%)	294 (96%)	11 (4%)	31	58
1	B	305/306 (100%)	289 (95%)	16 (5%)	21	42
All	All	610/612 (100%)	583 (96%)	27 (4%)	25	50

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	41	LYS
1	A	158	ARG
1	A	184	ASN
1	A	213	LEU
1	A	286	THR
1	A	289	ARG
1	A	333	GLU
1	A	342	GLU
1	A	359	ASN
1	A	361	SER
1	B	6	PRO
1	B	20	THR
1	B	34	ASP
1	B	37	GLU
1	B	44	GLU
1	B	67	ARG
1	B	68	GLU
1	B	149	ASP
1	B	185	GLU
1	B	213	LEU

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Mol	Chain	Res	Type
1	B	235	LEU
1	B	254	ASP
1	B	286	THR
1	B	309	LYS
1	B	333	GLU
1	B	370	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	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	174	ASN
1	B	221	GLN
1	B	384	GLN

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 oligosaccharides 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	XYL	A	400	3	9,9,9	0.89	0	11,11,11	1.91	3 (27%)
2	XYL	B	400	3	9,9,9	0.95	1 (11%)	11,11,11	1.35	1 (9%)

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	400	3	-	2/12/12/12	-
2	XYL	B	400	3	-	0/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	XYL	O3-C3	2.27	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	XYL	C5-C4-C3	4.24	120.82	112.17
2	B	400	XYL	O5-C5-C4	-3.14	104.56	111.16
2	A	400	XYL	O4-C4-C5	2.81	115.41	109.03
2	A	400	XYL	O2-C2-C1	-2.13	104.19	109.03

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	XYL	O3-C3-C4-C5
2	A	400	XYL	C2-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 [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.