



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:37 PM UTC

PDB ID : 1XLJ / pdb_00001xlj
Title : MECHANISM FOR ALDOSE-KETOSE INTERCONVERSION BY D-XYLOSE ISOMERASE INVOLVING RING OPENING FOLLOWED BY A 1,2-HYDRIDE SHIFT
Authors : Collyer, C.A.; Henrick, K.; Blow, D.M.
Deposited on : 1991-10-09
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

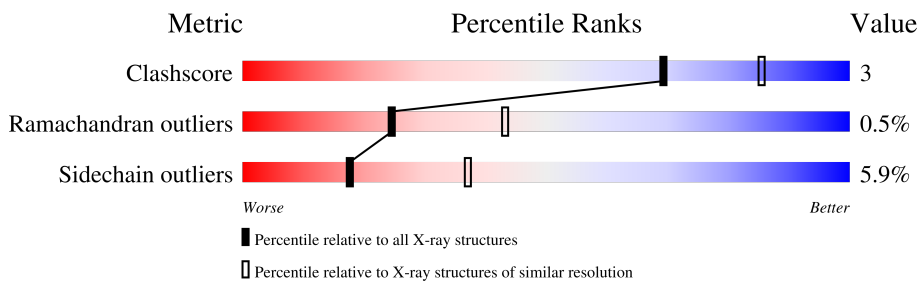
1 Overall quality at a glance

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	394	
1	B	394	

2 Entry composition [i](#)

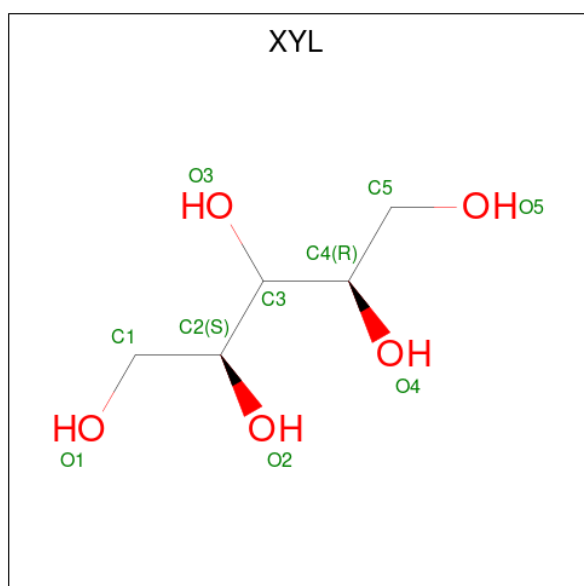
There are 4 unique types of molecules in this entry. The entry contains 6590 atoms, of which 0 are hydrogens and 0 are deuteriums.

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			

- 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 MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is water.

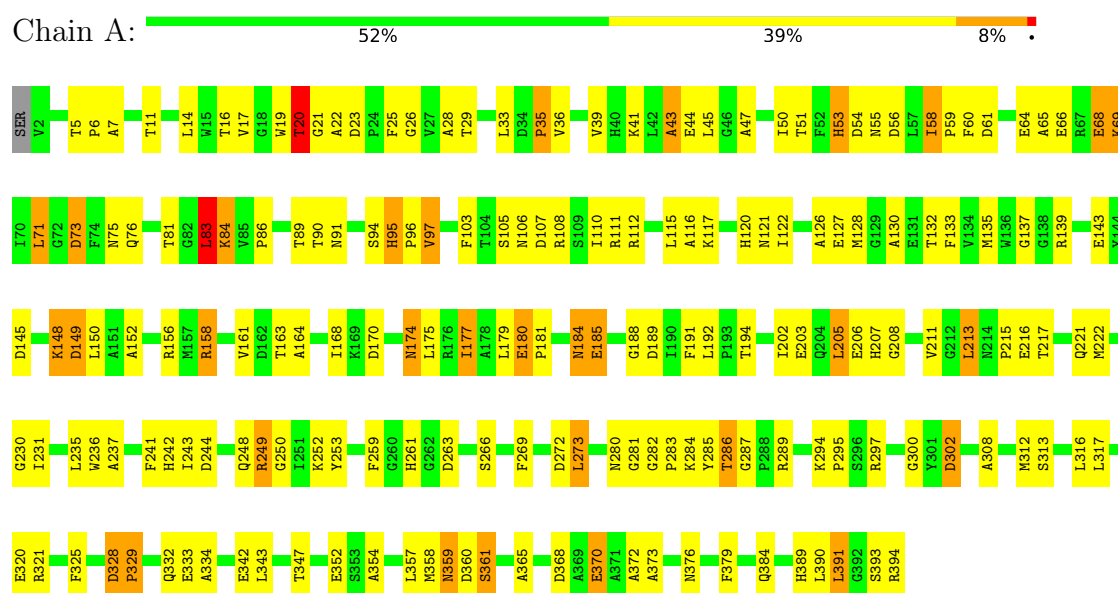
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	256	Total 256	O 256	0	0
4	B	258	Total 258	O 258	0	0

3 Residue-property plots

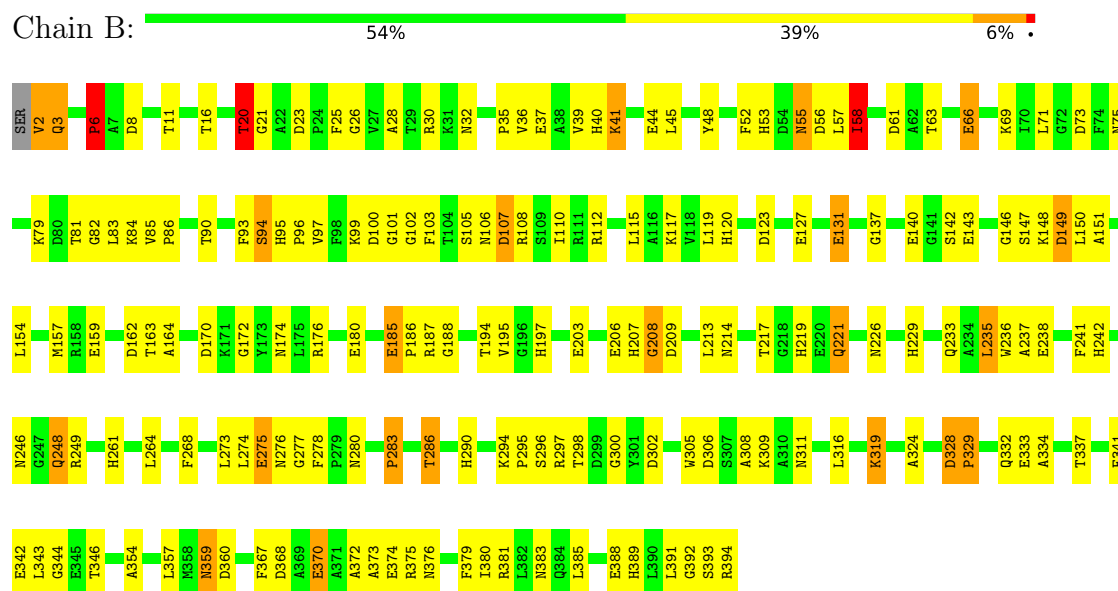
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.156 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6590	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: MN, 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	1.39	4/3101 (0.1%)	2.67	308/4204 (7.3%)
1	B	1.43	11/3101 (0.4%)	2.61	238/4204 (5.7%)
All	All	1.41	15/6202 (0.2%)	2.64	546/8408 (6.5%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	GLY	CA-C	6.98	1.56	1.51
1	B	286	THR	CA-CB	6.20	1.62	1.53
1	B	373	ALA	C-O	6.17	1.31	1.24
1	B	81	THR	CA-CB	5.60	1.62	1.53
1	A	149	ASP	CA-C	5.60	1.59	1.52
1	B	16	THR	C-O	5.58	1.29	1.23
1	B	20	THR	C-O	5.51	1.31	1.24
1	B	372	ALA	C-O	5.51	1.30	1.24
1	A	20	THR	CA-C	-5.39	1.45	1.52
1	B	233	GLN	C-O	5.37	1.30	1.24
1	B	277	GLY	N-CA	5.24	1.53	1.45
1	B	101	GLY	C-N	-5.23	1.29	1.33
1	B	16	THR	CA-CB	5.22	1.60	1.53
1	A	300	GLY	N-CA	5.19	1.51	1.45
1	A	282	GLY	N-CA	5.18	1.51	1.44

All (546) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	359	ASN	CA-CB-CG	21.86	134.46	112.60
1	A	6	PRO	CA-C-N	15.48	143.84	120.31
1	A	6	PRO	C-N-CA	15.48	143.84	120.31
1	B	379	PHE	CA-CB-CG	14.37	128.17	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	ASN	CA-CB-CG	-13.77	98.83	112.60
1	A	358	MET	CA-C-N	13.29	139.16	120.29
1	A	358	MET	C-N-CA	13.29	139.16	120.29
1	B	112	ARG	CD-NE-CZ	13.15	142.81	124.40
1	B	73	ASP	CA-CB-CG	12.72	125.32	112.60
1	B	343	LEU	CA-C-N	11.45	134.76	120.22
1	B	343	LEU	C-N-CA	11.45	134.76	120.22
1	B	372	ALA	O-C-N	-11.04	110.42	122.12
1	A	137	GLY	CA-C-N	10.95	133.83	120.14
1	A	137	GLY	C-N-CA	10.95	133.83	120.14
1	A	379	PHE	CA-CB-CG	10.89	124.69	113.80
1	B	20	THR	N-CA-CB	-10.51	93.96	110.46
1	B	392	GLY	CA-C-N	10.16	134.26	120.44
1	B	392	GLY	C-N-CA	10.16	134.26	120.44
1	A	393	SER	CA-C-N	9.98	139.67	121.70
1	A	393	SER	C-N-CA	9.98	139.67	121.70
1	A	103	PHE	CA-CB-CG	9.86	123.66	113.80
1	B	208	GLY	CA-C-N	9.86	133.88	120.38
1	B	208	GLY	C-N-CA	9.86	133.88	120.38
1	A	161	VAL	CA-C-O	-9.68	110.91	121.17
1	A	342	GLU	CA-CB-CG	9.66	133.41	114.10
1	B	117	LYS	CA-C-N	9.53	132.76	120.56
1	B	117	LYS	C-N-CA	9.53	132.76	120.56
1	B	26	GLY	N-CA-C	9.42	126.20	110.56
1	B	332	GLN	CA-C-N	9.33	132.57	120.44
1	B	332	GLN	C-N-CA	9.33	132.57	120.44
1	A	65	ALA	N-CA-C	-9.27	101.13	111.14
1	A	302	ASP	CA-C-N	9.27	130.26	119.98
1	A	302	ASP	C-N-CA	9.27	130.26	119.98
1	A	281	GLY	CA-C-O	-9.17	114.13	122.57
1	A	6	PRO	O-C-N	-9.13	110.31	122.64
1	A	343	LEU	CA-C-N	9.11	137.00	120.79
1	A	343	LEU	C-N-CA	9.11	137.00	120.79
1	A	14	LEU	CA-C-N	8.99	135.74	120.72
1	A	14	LEU	C-N-CA	8.99	135.74	120.72
1	A	222	MET	CA-C-N	8.98	136.41	122.49
1	A	222	MET	C-N-CA	8.98	136.41	122.49
1	A	73	ASP	CA-CB-CG	8.96	121.56	112.60
1	A	163	THR	CA-C-N	8.93	132.25	120.28
1	A	163	THR	C-N-CA	8.93	132.25	120.28
1	B	368	ASP	CA-CB-CG	8.78	121.38	112.60
1	B	20	THR	CB-CA-C	8.78	126.57	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ALA	CA-C-N	8.77	132.03	120.28
1	A	334	ALA	C-N-CA	8.77	132.03	120.28
1	A	235	LEU	CA-C-N	8.72	132.33	120.38
1	A	235	LEU	C-N-CA	8.72	132.33	120.38
1	B	319	LYS	CA-C-N	8.64	131.67	120.44
1	B	319	LYS	C-N-CA	8.64	131.67	120.44
1	B	23	ASP	CB-CA-C	8.63	127.17	110.17
1	B	302	ASP	CA-C-N	8.61	129.47	120.00
1	B	302	ASP	C-N-CA	8.61	129.47	120.00
1	A	372	ALA	O-C-N	-8.55	112.41	122.15
1	A	149	ASP	N-CA-C	-8.48	94.76	108.41
1	A	357	LEU	CA-C-O	-8.46	111.99	120.70
1	B	102	GLY	N-CA-C	-8.43	102.54	110.21
1	B	334	ALA	CA-C-N	8.39	131.35	120.44
1	B	334	ALA	C-N-CA	8.39	131.35	120.44
1	B	106	ASN	OD1-CG-ND2	-8.36	114.24	122.60
1	A	51	THR	CA-CB-CG2	8.34	124.68	110.50
1	B	127	GLU	CA-CB-CG	8.33	130.75	114.10
1	A	149	ASP	N-CA-CB	8.32	123.44	110.21
1	A	394	ARG	CD-NE-CZ	8.31	136.04	124.40
1	A	60	PHE	CA-CB-CG	8.30	122.10	113.80
1	B	275	GLU	CA-C-N	8.29	136.78	121.52
1	B	275	GLU	C-N-CA	8.29	136.78	121.52
1	B	207	HIS	CA-C-N	8.29	130.57	120.13
1	B	207	HIS	C-N-CA	8.29	130.57	120.13
1	A	370	GLU	CA-C-O	-8.26	111.66	120.42
1	A	26	GLY	N-CA-C	8.24	123.18	110.91
1	A	235	LEU	O-C-N	-8.23	113.59	122.07
1	A	342	GLU	N-CA-CB	8.18	122.82	110.22
1	A	180	GLU	CA-C-O	8.15	127.28	119.62
1	B	333	GLU	CA-C-N	8.03	131.04	120.28
1	B	333	GLU	C-N-CA	8.03	131.04	120.28
1	B	241	PHE	CA-CB-CG	8.00	121.80	113.80
1	B	53	HIS	N-CA-CB	7.95	123.64	110.52
1	A	352	GLU	CA-C-O	-7.95	111.78	120.36
1	A	43	ALA	O-C-N	-7.92	113.73	122.12
1	A	263	ASP	CA-CB-CG	7.87	120.47	112.60
1	A	203	GLU	CB-CG-CD	7.81	125.88	112.60
1	B	55	ASN	CA-C-N	7.81	131.38	120.29
1	B	55	ASN	C-N-CA	7.81	131.38	120.29
1	A	312	MET	CA-C-N	7.79	130.56	120.44
1	A	312	MET	C-N-CA	7.79	130.56	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	PHE	CA-CB-CG	7.78	121.58	113.80
1	A	19	TRP	CA-C-N	7.77	136.73	121.58
1	A	19	TRP	C-N-CA	7.77	136.73	121.58
1	B	283	PRO	CB-CA-C	7.73	121.08	110.95
1	B	2	VAL	CA-C-N	7.71	140.61	121.80
1	B	2	VAL	C-N-CA	7.71	140.61	121.80
1	A	174	ASN	N-CA-CB	7.71	123.32	110.53
1	B	286	THR	N-CA-CB	-7.67	98.64	110.92
1	A	320	GLU	CA-CB-CG	7.65	129.41	114.10
1	B	143	GLU	CA-C-O	7.62	128.02	119.41
1	B	298	THR	CA-C-N	7.62	134.00	122.65
1	B	298	THR	C-N-CA	7.62	134.00	122.65
1	A	250	GLY	N-CA-C	7.61	122.82	112.17
1	A	194	THR	CA-CB-CG2	7.58	123.38	110.50
1	A	91	ASN	CB-CG-ND2	-7.57	105.04	116.40
1	A	14	LEU	O-C-N	-7.56	114.11	122.12
1	A	221	GLN	CA-C-N	7.49	136.02	121.18
1	A	221	GLN	C-N-CA	7.49	136.02	121.18
1	B	324	ALA	CA-C-N	7.48	130.52	120.65
1	B	324	ALA	C-N-CA	7.48	130.52	120.65
1	A	139	ARG	NE-CZ-NH2	7.44	125.90	119.20
1	B	187	ARG	NE-CZ-NH2	-7.42	112.52	119.20
1	B	242	HIS	CA-CB-CG	7.41	121.21	113.80
1	A	208	GLY	O-C-N	-7.38	114.46	122.73
1	A	272	ASP	CA-C-N	7.36	130.00	120.44
1	A	272	ASP	C-N-CA	7.36	130.00	120.44
1	B	44	GLU	N-CA-CB	7.35	120.93	110.12
1	A	376	ASN	OD1-CG-ND2	-7.30	115.30	122.60
1	B	381	ARG	NE-CZ-NH2	-7.29	112.64	119.20
1	A	23	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	94	SER	N-CA-C	7.23	120.59	111.69
1	B	391	LEU	CA-C-N	7.23	135.12	120.80
1	B	391	LEU	C-N-CA	7.23	135.12	120.80
1	A	163	THR	CA-CB-CG2	7.22	122.77	110.50
1	A	269	PHE	CA-C-O	-7.21	111.67	119.97
1	B	106	ASN	CA-C-N	7.21	131.62	121.24
1	B	106	ASN	C-N-CA	7.21	131.62	121.24
1	B	56	ASP	N-CA-CB	7.20	120.82	110.16
1	B	206	GLU	CA-CB-CG	7.20	128.50	114.10
1	A	96	PRO	O-C-N	-7.19	113.47	122.17
1	B	131	GLU	CB-CG-CD	7.14	124.74	112.60
1	B	99	LYS	CA-C-O	-7.14	110.85	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	PHE	CA-C-N	7.14	127.46	119.32
1	B	278	PHE	C-N-CA	7.14	127.46	119.32
1	B	297	ARG	NE-CZ-NH2	7.13	125.62	119.20
1	A	106	ASN	CA-C-N	7.11	132.58	121.99
1	A	106	ASN	C-N-CA	7.11	132.58	121.99
1	B	120	HIS	CA-C-N	7.11	131.11	120.31
1	B	120	HIS	C-N-CA	7.11	131.11	120.31
1	B	388	GLU	O-C-N	-7.08	114.61	122.12
1	B	94	SER	N-CA-C	7.05	120.37	111.69
1	B	207	HIS	CA-CB-CG	-7.05	106.75	113.80
1	A	359	ASN	CA-C-O	-7.02	112.98	120.42
1	B	20	THR	CA-CB-CG2	7.02	122.43	110.50
1	B	214	ASN	OD1-CG-ND2	-7.01	115.58	122.60
1	A	249	ARG	CD-NE-CZ	7.01	134.22	124.40
1	B	96	PRO	CA-C-N	7.00	131.53	120.47
1	B	96	PRO	C-N-CA	7.00	131.53	120.47
1	B	20	THR	CA-C-O	6.99	127.50	119.18
1	A	283	PRO	CB-CA-C	6.98	120.12	111.12
1	A	203	GLU	CA-C-N	6.97	134.04	122.54
1	A	203	GLU	C-N-CA	6.97	134.04	122.54
1	B	142	SER	CA-C-O	-6.96	114.00	121.38
1	B	308	ALA	CA-C-N	6.95	129.48	120.44
1	B	308	ALA	C-N-CA	6.95	129.48	120.44
1	B	372	ALA	CB-CA-C	6.94	122.32	110.79
1	A	20	THR	CA-CB-CG2	6.94	122.30	110.50
1	A	112	ARG	NE-CZ-NH1	6.94	128.44	121.50
1	A	143	GLU	CA-C-O	6.91	127.22	119.41
1	A	316	LEU	CB-CA-C	6.91	122.26	110.79
1	B	328	ASP	CA-C-N	6.90	127.19	119.32
1	B	328	ASP	C-N-CA	6.90	127.19	119.32
1	A	236	TRP	O-C-N	-6.89	114.81	122.12
1	A	237	ALA	CA-C-N	6.89	132.55	122.63
1	A	237	ALA	C-N-CA	6.89	132.55	122.63
1	A	36	VAL	O-C-N	6.89	128.66	121.91
1	A	55	ASN	CA-CB-CG	6.88	119.47	112.60
1	A	259	PHE	CA-C-N	6.84	133.25	122.51
1	A	259	PHE	C-N-CA	6.84	133.25	122.51
1	A	84	LYS	CB-CA-C	6.80	121.01	109.80
1	B	84	LYS	N-CA-C	-6.79	100.74	110.59
1	B	149	ASP	N-CA-C	-6.79	96.58	108.20
1	A	354	ALA	CA-C-N	6.78	129.69	120.54
1	A	354	ALA	C-N-CA	6.78	129.69	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	PRO	O-C-N	-6.77	113.98	122.17
1	A	95	HIS	CA-C-N	6.76	127.31	119.47
1	A	95	HIS	C-N-CA	6.76	127.31	119.47
1	A	235	LEU	CA-C-O	6.74	127.90	120.82
1	A	302	ASP	CA-CB-CG	-6.73	105.87	112.60
1	B	217	THR	CA-C-N	6.72	127.56	120.03
1	B	217	THR	C-N-CA	6.72	127.56	120.03
1	B	219	HIS	CB-CG-CD2	6.72	139.94	131.20
1	A	170	ASP	CA-C-O	-6.70	113.45	120.55
1	A	244	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	127	GLU	CA-CB-CG	6.67	127.43	114.10
1	A	289	ARG	CD-NE-CZ	6.67	133.73	124.40
1	A	308	ALA	CA-C-O	6.66	127.82	120.82
1	B	380	ILE	N-CA-CB	6.66	118.34	110.55
1	B	221	GLN	CA-C-N	6.66	131.83	120.72
1	B	221	GLN	C-N-CA	6.66	131.83	120.72
1	B	146	GLY	CA-C-N	6.65	131.83	120.72
1	B	146	GLY	C-N-CA	6.65	131.83	120.72
1	A	243	ILE	O-C-N	6.65	130.80	123.09
1	B	174	ASN	CA-C-N	6.65	133.26	122.29
1	B	174	ASN	C-N-CA	6.65	133.26	122.29
1	B	209	ASP	CA-CB-CG	6.65	119.25	112.60
1	B	367	PHE	CA-C-N	-6.64	113.61	122.85
1	B	367	PHE	C-N-CA	-6.64	113.61	122.85
1	B	93	PHE	CA-C-O	-6.63	111.03	120.51
1	A	14	LEU	CA-C-O	6.58	127.53	120.55
1	A	389	HIS	N-CA-CB	6.57	119.60	110.07
1	B	75	ASN	OD1-CG-ND2	6.57	129.17	122.60
1	B	159	GLU	CA-CB-CG	6.57	127.23	114.10
1	B	108	ARG	NE-CZ-NH2	-6.55	113.30	119.20
1	A	243	ILE	CA-C-O	-6.54	113.91	120.90
1	B	296	SER	CA-C-O	6.53	128.34	121.15
1	A	370	GLU	CB-CG-CD	6.53	123.70	112.60
1	A	127	GLU	N-CA-CB	6.53	119.66	109.94
1	A	121	ASN	CA-C-N	6.52	128.78	120.56
1	A	121	ASN	C-N-CA	6.52	128.78	120.56
1	A	213	LEU	CD1-CG-CD2	-6.49	96.51	110.80
1	A	56	ASP	CA-CB-CG	6.48	119.08	112.60
1	B	359	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	A	286	THR	CA-C-O	-6.46	111.56	119.18
1	A	56	ASP	N-CA-C	-6.45	104.33	111.36
1	B	56	ASP	N-CA-C	-6.45	104.33	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	ASP	CA-C-N	6.44	129.16	120.65
1	A	263	ASP	C-N-CA	6.44	129.16	120.65
1	B	164	ALA	CA-C-N	6.43	129.19	120.44
1	B	164	ALA	C-N-CA	6.43	129.19	120.44
1	B	40	HIS	CA-CB-CG	-6.42	107.38	113.80
1	B	264	LEU	N-CA-C	6.41	118.27	111.28
1	A	117	LYS	CA-C-N	6.41	128.54	120.72
1	A	117	LYS	C-N-CA	6.41	128.54	120.72
1	A	285	TYR	CA-C-N	-6.41	112.30	122.29
1	A	285	TYR	C-N-CA	-6.41	112.30	122.29
1	A	207	HIS	O-C-N	-6.38	114.11	122.59
1	A	53	HIS	N-CA-CB	6.36	121.02	110.52
1	B	8	ASP	CA-C-N	6.33	131.12	122.19
1	B	8	ASP	C-N-CA	6.33	131.12	122.19
1	B	127	GLU	CA-C-N	6.33	129.93	120.31
1	B	127	GLU	C-N-CA	6.33	129.93	120.31
1	A	83	LEU	CB-CA-C	6.32	120.46	109.65
1	B	268	PHE	CA-C-N	6.32	129.38	120.28
1	B	268	PHE	C-N-CA	6.32	129.38	120.28
1	A	44	GLU	N-CA-CB	6.31	119.39	110.12
1	A	59	PRO	CB-CA-C	6.28	119.43	111.39
1	B	52	PHE	CA-C-O	6.28	127.95	121.23
1	A	84	LYS	O-C-N	-6.28	115.94	123.03
1	B	36	VAL	CB-CA-C	6.27	120.88	112.22
1	A	297	ARG	CA-C-N	6.27	131.34	120.68
1	A	297	ARG	C-N-CA	6.27	131.34	120.68
1	B	342	GLU	CG-CD-OE2	-6.27	103.98	118.40
1	B	391	LEU	O-C-N	-6.27	113.81	122.46
1	A	7	ALA	CA-C-N	6.25	129.81	120.31
1	A	7	ALA	C-N-CA	6.25	129.81	120.31
1	A	115	LEU	CA-C-N	6.25	128.57	120.44
1	A	115	LEU	C-N-CA	6.25	128.57	120.44
1	A	23	ASP	CB-CG-OD1	6.25	132.77	118.40
1	A	116	ALA	CA-C-N	6.23	128.63	120.28
1	A	116	ALA	C-N-CA	6.23	128.63	120.28
1	B	290	HIS	CA-CB-CG	6.22	120.02	113.80
1	A	329	PRO	CA-C-N	6.21	128.61	120.28
1	A	329	PRO	C-N-CA	6.21	128.61	120.28
1	B	203	GLU	CG-CD-OE2	6.21	132.69	118.40
1	A	164	ALA	CA-C-N	6.21	131.20	120.58
1	A	164	ALA	C-N-CA	6.21	131.20	120.58
1	B	197	HIS	CA-CB-CG	-6.21	107.59	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	PRO	CA-C-N	6.20	129.27	120.53
1	A	96	PRO	C-N-CA	6.20	129.27	120.53
1	B	342	GLU	CB-CG-CD	6.18	123.10	112.60
1	B	172	GLY	CA-C-O	-6.16	112.64	120.03
1	B	194	THR	CA-CB-CG2	6.16	120.97	110.50
1	B	233	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	A	230	GLY	O-C-N	-6.14	116.29	122.19
1	A	320	GLU	CA-C-N	6.14	128.42	120.44
1	A	320	GLU	C-N-CA	6.14	128.42	120.44
1	A	189	ASP	CA-C-O	-6.14	112.73	120.28
1	A	359	ASN	CA-CB-CG	6.14	118.74	112.60
1	A	205	LEU	CA-C-O	6.13	127.97	120.92
1	B	115	LEU	CB-CA-C	6.13	120.50	110.88
1	A	120	HIS	CA-C-N	6.12	129.10	120.28
1	A	120	HIS	C-N-CA	6.12	129.10	120.28
1	B	163	THR	CA-CB-OG1	-6.12	100.42	109.60
1	A	54	ASP	CA-C-O	-6.12	114.07	120.92
1	A	71	LEU	CA-C-N	6.12	126.73	120.00
1	A	71	LEU	C-N-CA	6.12	126.73	120.00
1	A	253	TYR	CA-C-O	-6.10	115.08	121.55
1	B	48	TYR	N-CA-CB	-6.10	101.56	110.47
1	B	388	GLU	CA-C-N	6.10	128.74	120.44
1	B	388	GLU	C-N-CA	6.10	128.74	120.44
1	A	107	ASP	CA-C-O	6.10	127.49	120.60
1	A	332	GLN	CB-CG-CD	6.09	122.96	112.60
1	A	391	LEU	CA-C-N	6.08	133.34	121.41
1	A	391	LEU	C-N-CA	6.08	133.34	121.41
1	A	53	HIS	CB-CA-C	-6.08	99.26	109.48
1	B	342	GLU	O-C-N	-6.08	115.27	122.20
1	A	54	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	280	ASN	OD1-CG-ND2	-6.06	116.54	122.60
1	A	59	PRO	CA-C-N	6.05	128.31	120.44
1	A	59	PRO	C-N-CA	6.05	128.31	120.44
1	B	147	SER	CA-C-N	6.05	132.02	122.21
1	B	147	SER	C-N-CA	6.05	132.02	122.21
1	A	177	ILE	O-C-N	6.05	129.85	122.95
1	A	295	PRO	CA-C-O	-6.04	114.93	121.27
1	A	168	ILE	CA-C-N	6.03	128.28	120.44
1	A	168	ILE	C-N-CA	6.03	128.28	120.44
1	A	216	GLU	CA-C-N	6.03	129.17	120.79
1	A	216	GLU	C-N-CA	6.03	129.17	120.79
1	B	37	GLU	CA-C-N	6.03	129.17	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	GLU	C-N-CA	6.03	129.17	120.79
1	B	370	GLU	CA-C-O	-6.02	113.29	120.10
1	B	337	THR	CA-CB-OG1	-6.02	100.57	109.60
1	A	110	ILE	O-C-N	-6.01	116.02	121.91
1	A	106	ASN	CA-CB-CG	5.98	118.58	112.60
1	A	120	HIS	O-C-N	-5.97	115.88	122.09
1	A	266	SER	CA-C-N	5.97	128.20	120.44
1	A	266	SER	C-N-CA	5.97	128.20	120.44
1	B	237	ALA	CA-C-N	5.97	130.63	122.34
1	B	237	ALA	C-N-CA	5.97	130.63	122.34
1	B	53	HIS	CA-CB-CG	5.96	119.77	113.80
1	A	342	GLU	CA-C-O	-5.96	113.37	120.10
1	B	248	GLN	OE1-CD-NE2	-5.95	116.65	122.60
1	A	360	ASP	CA-C-N	5.95	128.25	120.28
1	A	360	ASP	C-N-CA	5.95	128.25	120.28
1	A	342	GLU	CB-CA-C	-5.94	99.64	110.63
1	B	170	ASP	O-C-N	-5.91	115.95	122.09
1	B	213	LEU	CA-CB-CG	5.91	136.97	116.30
1	A	343	LEU	O-C-N	-5.90	115.31	122.22
1	B	32	ASN	CA-C-O	-5.90	115.29	121.55
1	B	188	GLY	CA-C-N	5.90	131.12	122.39
1	B	188	GLY	C-N-CA	5.90	131.12	122.39
1	A	156	ARG	CA-C-N	5.90	128.11	120.44
1	A	156	ARG	C-N-CA	5.90	128.11	120.44
1	A	66	GLU	CA-C-N	5.89	128.10	120.44
1	A	66	GLU	C-N-CA	5.89	128.10	120.44
1	A	20	THR	N-CA-CB	-5.88	100.53	110.41
1	B	119	LEU	CA-C-N	5.88	128.16	120.28
1	B	119	LEU	C-N-CA	5.88	128.16	120.28
1	B	360	ASP	CA-C-O	5.87	127.03	120.92
1	A	133	PHE	CA-C-O	5.87	126.56	120.40
1	A	273	LEU	CA-C-O	-5.87	114.66	120.82
1	A	221	GLN	O-C-N	-5.86	114.58	122.43
1	A	352	GLU	N-CA-C	-5.86	99.35	108.90
1	A	56	ASP	CA-C-N	5.84	129.83	121.71
1	A	56	ASP	C-N-CA	5.84	129.83	121.71
1	B	333	GLU	O-C-N	-5.84	116.05	122.07
1	A	188	GLY	CA-C-O	-5.84	114.47	120.66
1	B	393	SER	CA-C-O	-5.83	114.70	120.70
1	A	261	HIS	CA-C-N	5.81	132.79	121.41
1	A	261	HIS	C-N-CA	5.81	132.79	121.41
1	B	236	TRP	CA-CB-CG	5.80	124.62	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ASN	CA-CB-CG	-5.79	106.81	112.60
1	B	385	LEU	CA-C-O	-5.79	114.41	120.55
1	A	68	GLU	CB-CG-CD	-5.79	102.76	112.60
1	A	120	HIS	CA-CB-CG	-5.79	108.01	113.80
1	A	328	ASP	CA-C-O	5.79	125.22	119.49
1	A	21	GLY	N-CA-C	5.77	123.41	115.27
1	A	249	ARG	NE-CZ-NH1	5.77	127.27	121.50
1	A	97	VAL	N-CA-CB	5.76	117.67	110.47
1	A	325	PHE	CA-CB-CG	5.75	119.55	113.80
1	A	211	VAL	CB-CA-C	5.75	119.39	110.83
1	A	390	LEU	N-CA-C	5.74	117.54	111.28
1	B	176	ARG	CB-CG-CD	5.74	124.50	111.30
1	A	393	SER	N-CA-C	-5.74	105.61	113.30
1	B	195	VAL	CA-C-N	5.74	126.47	119.99
1	B	195	VAL	C-N-CA	5.74	126.47	119.99
1	A	368	ASP	CA-C-N	5.73	128.23	120.38
1	A	368	ASP	C-N-CA	5.73	128.23	120.38
1	A	91	ASN	CB-CG-OD1	5.72	132.24	120.80
1	A	75	ASN	CA-CB-CG	5.72	118.32	112.60
1	A	61	ASP	CA-C-O	-5.71	112.36	119.28
1	B	246	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	A	111	ARG	CA-C-N	5.70	127.85	120.44
1	A	111	ARG	C-N-CA	5.70	127.85	120.44
1	B	283	PRO	CA-C-O	5.69	129.37	122.08
1	B	379	PHE	CB-CA-C	5.69	121.99	110.38
1	B	163	THR	CA-C-O	-5.69	114.84	120.70
1	A	81	THR	N-CA-C	5.67	120.26	113.23
1	A	20	THR	CB-CA-C	5.66	121.22	109.95
1	A	105	SER	N-CA-C	-5.66	102.65	110.35
1	B	56	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	361	SER	CA-C-N	5.65	127.85	120.28
1	A	361	SER	C-N-CA	5.65	127.85	120.28
1	A	361	SER	N-CA-C	5.65	117.44	111.28
1	B	75	ASN	CA-CB-CG	-5.64	106.96	112.60
1	B	21	GLY	CA-C-N	-5.64	113.44	121.50
1	B	21	GLY	C-N-CA	-5.64	113.44	121.50
1	A	51	THR	CA-CB-OG1	-5.64	101.14	109.60
1	B	100	ASP	CB-CA-C	5.64	120.24	110.72
1	A	174	ASN	OD1-CG-ND2	5.63	128.24	122.60
1	B	137	GLY	CA-C-N	5.63	127.38	120.22
1	B	137	GLY	C-N-CA	5.63	127.38	120.22
1	B	180	GLU	CA-C-O	5.63	124.91	119.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	PRO	CA-C-O	-5.61	115.02	121.86
1	A	206	GLU	N-CA-CB	5.60	118.45	110.16
1	B	389	HIS	N-CA-CB	5.60	118.20	110.07
1	B	296	SER	CA-C-N	5.59	129.55	120.60
1	B	296	SER	C-N-CA	5.59	129.55	120.60
1	A	145	ASP	CA-C-O	-5.59	113.55	119.97
1	B	346	THR	CA-CB-OG1	-5.58	101.22	109.60
1	A	152	ALA	CA-C-O	-5.58	113.56	119.97
1	A	320	GLU	CG-CD-OE2	5.57	131.22	118.40
1	A	29	THR	CA-C-O	5.56	125.17	119.05
1	A	202	ILE	CA-C-N	5.56	131.33	120.99
1	A	202	ILE	C-N-CA	5.56	131.33	120.99
1	A	16	THR	O-C-N	-5.55	115.56	122.11
1	B	261	HIS	CA-C-N	5.55	132.30	121.41
1	B	261	HIS	C-N-CA	5.55	132.30	121.41
1	B	25	PHE	CA-CB-CG	-5.55	108.25	113.80
1	A	217	THR	CA-C-N	5.54	126.10	120.00
1	A	217	THR	C-N-CA	5.54	126.10	120.00
1	A	81	THR	CA-CB-OG1	-5.54	101.29	109.60
1	B	66	GLU	CB-CA-C	-5.54	102.19	110.88
1	B	150	LEU	CB-CA-C	5.53	119.97	110.79
1	A	188	GLY	N-CA-C	-5.52	105.70	112.77
1	A	389	HIS	CA-CB-CG	-5.52	108.28	113.80
1	A	33	LEU	CA-C-O	-5.52	114.45	120.36
1	A	47	ALA	CA-C-O	5.51	127.39	121.44
1	A	23	ASP	CB-CA-C	5.50	121.01	110.17
1	B	383	ASN	CA-C-N	5.49	127.90	120.38
1	B	383	ASN	C-N-CA	5.49	127.90	120.38
1	A	365	ALA	CA-C-O	-5.48	115.03	120.90
1	A	107	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	102	GLY	CA-C-N	5.47	128.37	120.38
1	B	102	GLY	C-N-CA	5.47	128.37	120.38
1	B	238	GLU	CA-CB-CG	-5.47	103.15	114.10
1	B	108	ARG	CD-NE-CZ	5.47	132.06	124.40
1	A	213	LEU	N-CA-C	5.46	118.60	110.14
1	A	94	SER	CA-C-O	-5.46	114.18	120.24
1	A	112	ARG	CD-NE-CZ	5.45	132.03	124.40
1	A	390	LEU	CA-C-N	5.45	132.24	122.38
1	A	390	LEU	C-N-CA	5.45	132.24	122.38
1	A	297	ARG	N-CA-C	5.43	119.39	112.87
1	A	248	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	B	162	ASP	CA-CB-CG	5.42	118.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	LEU	O-C-N	5.41	129.88	123.33
1	A	221	GLN	N-CA-CB	-5.40	101.42	110.39
1	B	101	GLY	O-C-N	5.40	128.48	123.35
1	A	269	PHE	CA-C-N	5.39	127.78	120.44
1	A	269	PHE	C-N-CA	5.39	127.78	120.44
1	B	172	GLY	O-C-N	5.39	127.48	122.57
1	A	115	LEU	CB-CA-C	5.38	119.73	110.79
1	B	106	ASN	N-CA-CB	5.38	118.62	110.28
1	A	313	SER	N-CA-CB	-5.38	102.22	110.01
1	A	19	TRP	CA-C-O	5.37	126.81	120.58
1	B	300	GLY	O-C-N	-5.37	118.19	122.81
1	A	368	ASP	OD1-CG-OD2	-5.36	110.03	122.90
1	B	63	THR	CA-CB-OG1	-5.36	101.56	109.60
1	A	372	ALA	CA-C-O	5.35	126.10	120.42
1	A	231	ILE	CB-CA-C	5.35	120.93	112.26
1	B	123	ASP	OD1-CG-OD2	-5.35	110.07	122.90
1	B	280	ASN	CA-C-O	-5.33	113.11	119.35
1	B	75	ASN	CA-C-N	5.33	127.37	120.44
1	B	75	ASN	C-N-CA	5.33	127.37	120.44
1	A	65	ALA	CA-C-O	-5.33	115.21	120.70
1	B	238	GLU	CG-CD-OE2	5.32	130.64	118.40
1	B	311	ASN	CA-C-N	5.32	127.68	120.44
1	B	311	ASN	C-N-CA	5.32	127.68	120.44
1	B	332	GLN	OE1-CD-NE2	-5.32	117.28	122.60
1	A	128	MET	N-CA-C	5.32	119.25	112.87
1	A	17	VAL	CA-C-O	5.32	126.44	119.85
1	B	274	LEU	O-C-N	5.32	128.21	122.15
1	A	156	ARG	CA-CB-CG	5.31	124.72	114.10
1	B	82	GLY	CA-C-O	-5.30	113.13	119.06
1	A	90	THR	CA-C-N	-5.29	115.97	122.84
1	A	90	THR	C-N-CA	-5.29	115.97	122.84
1	A	25	PHE	CA-C-N	5.29	128.81	121.09
1	A	25	PHE	C-N-CA	5.29	128.81	121.09
1	A	126	ALA	O-C-N	-5.28	116.63	122.07
1	A	130	ALA	CA-C-N	5.28	129.61	120.58
1	A	130	ALA	C-N-CA	5.28	129.61	120.58
1	A	148	LYS	N-CA-C	5.28	117.84	109.50
1	A	333	GLU	CA-C-N	5.28	127.35	120.28
1	A	333	GLU	C-N-CA	5.28	127.35	120.28
1	B	354	ALA	CA-C-N	5.27	128.11	120.79
1	B	354	ALA	C-N-CA	5.27	128.11	120.79
1	A	64	GLU	CA-C-N	5.26	127.59	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	GLU	C-N-CA	5.26	127.59	120.44
1	A	192	LEU	CA-C-N	5.26	124.87	119.56
1	A	192	LEU	C-N-CA	5.26	124.87	119.56
1	A	287	GLY	CA-C-O	5.26	129.04	121.52
1	B	333	GLU	N-CA-CB	-5.26	102.39	110.01
1	A	179	LEU	O-C-N	5.25	129.25	123.16
1	A	208	GLY	CA-C-N	5.25	127.83	120.28
1	A	208	GLY	C-N-CA	5.25	127.83	120.28
1	B	6	PRO	CA-C-O	-5.24	111.07	120.60
1	A	68	GLU	OE1-CD-OE2	5.24	135.46	122.90
1	A	35	PRO	CA-C-N	5.23	127.15	120.56
1	A	35	PRO	C-N-CA	5.23	127.15	120.56
1	A	384	GLN	CB-CG-CD	5.23	121.49	112.60
1	A	242	HIS	O-C-N	-5.23	117.77	123.26
1	B	105	SER	CA-C-O	-5.23	115.44	121.19
1	B	154	LEU	CA-C-O	-5.22	114.88	120.42
1	B	85	VAL	N-CA-CB	5.22	118.52	111.21
1	B	154	LEU	CB-CA-C	5.21	119.71	110.85
1	B	376	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	A	297	ARG	O-C-N	-5.20	115.51	122.43
1	A	241	PHE	CA-CB-CG	5.20	119.00	113.80
1	B	127	GLU	CG-CD-OE2	5.19	130.34	118.40
1	B	148	LYS	N-CA-C	5.19	117.08	109.24
1	A	132	THR	CA-C-O	5.18	126.20	120.71
1	B	368	ASP	CA-C-N	5.18	127.18	120.44
1	B	368	ASP	C-N-CA	5.18	127.18	120.44
1	B	214	ASN	CB-CG-ND2	5.18	124.17	116.40
1	B	372	ALA	CA-C-O	5.17	126.03	120.55
1	A	332	GLN	CA-C-N	5.17	127.16	120.44
1	A	332	GLN	C-N-CA	5.17	127.16	120.44
1	B	58	ILE	O-C-N	5.17	125.92	121.12
1	B	71	LEU	CA-C-N	5.16	125.57	119.94
1	B	71	LEU	C-N-CA	5.16	125.57	119.94
1	A	236	TRP	CA-C-N	5.16	132.26	121.94
1	A	236	TRP	C-N-CA	5.16	132.26	121.94
1	A	372	ALA	CA-C-N	5.16	130.59	120.99
1	A	372	ALA	C-N-CA	5.16	130.59	120.99
1	B	344	GLY	CA-C-O	-5.15	114.63	120.30
1	B	79	LYS	O-C-N	-5.15	116.57	122.08
1	B	341	PHE	N-CA-C	-5.14	105.36	111.69
1	B	306	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	211	VAL	CA-CB-CG2	5.14	119.13	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ARG	CD-NE-CZ	5.13	131.58	124.40
1	B	283	PRO	O-C-N	-5.13	116.74	123.00
1	B	376	ASN	CB-CG-ND2	5.13	124.09	116.40
1	B	373	ALA	N-CA-C	5.13	119.02	112.87
1	A	84	LYS	CA-C-N	5.12	131.61	122.13
1	A	84	LYS	C-N-CA	5.12	131.61	122.13
1	B	123	ASP	CB-CG-OD2	5.12	130.18	118.40
1	B	316	LEU	CB-CA-C	5.12	119.55	110.85
1	A	259	PHE	CA-C-O	5.11	126.74	120.92
1	A	76	GLN	CA-C-N	5.10	127.43	120.54
1	A	76	GLN	C-N-CA	5.10	127.43	120.54
1	A	68	GLU	CA-CB-CG	-5.09	103.93	114.10
1	B	30	ARG	NE-CZ-NH1	5.08	126.58	121.50
1	A	122	ILE	CA-C-N	5.08	127.85	120.79
1	A	122	ILE	C-N-CA	5.08	127.85	120.79
1	B	360	ASP	CA-C-N	5.08	127.34	120.38
1	B	360	ASP	C-N-CA	5.08	127.34	120.38
1	B	394	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	B	249	ARG	NE-CZ-NH1	5.07	126.57	121.50
1	B	151	ALA	O-C-N	-5.06	116.38	122.15
1	A	16	THR	CA-CB-OG1	-5.06	102.00	109.60
1	A	22	ALA	O-C-N	5.05	128.97	123.01
1	A	58	ILE	N-CA-C	5.05	112.55	107.55
1	A	139	ARG	NH1-CZ-NH2	-5.05	112.73	119.30
1	A	126	ALA	CB-CA-C	5.05	118.81	110.88
1	A	289	ARG	N-CA-C	-5.05	97.20	107.41
1	B	107	ASP	CA-CB-CG	-5.02	107.58	112.60
1	B	100	ASP	O-C-N	-5.02	116.27	122.25
1	A	108	ARG	N-CA-C	5.02	117.48	111.71
1	A	5	THR	CA-C-N	5.01	126.11	119.84
1	A	5	THR	C-N-CA	5.01	126.11	119.84
1	A	373	ALA	CA-C-N	5.01	129.91	121.14
1	A	373	ALA	C-N-CA	5.01	129.91	121.14
1	B	142	SER	N-CA-CB	-5.01	103.74	111.46
1	B	57	LEU	N-CA-CB	-5.01	102.43	110.19
1	B	203	GLU	CA-C-N	5.00	130.80	122.54
1	B	203	GLU	C-N-CA	5.00	130.80	122.54
1	A	347	THR	CA-CB-CG2	5.00	119.01	110.50

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	2882	20	1
1	B	3027	0	2882	21	1
2	A	10	0	11	0	0
2	B	10	0	10	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	256	0	0	2	1
4	B	258	0	0	1	0
All	All	6590	0	5785	41	2

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 (41) 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	1.34	0.75
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.71	0.71
1:B:95:HIS:HD2	1:B:97:VAL:H	1.39	0.70
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.63	0.64
1:B:140:GLU:HG3	1:B:157:MET:HE1	1.84	0.60
1:A:58:ILE:HD11	1:A:71:LEU:HD21	1.84	0.60
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.85	0.57
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.87	0.57
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.88	0.54
1:B:235:LEU:HD22	1:B:283:PRO:HB2	1.90	0.54
1:A:69:LYS:HE2	1:A:73:ASP:OD2	2.09	0.53
1:A:84:LYS:HD2	4:A:423(A):HOH:O	2.10	0.50
1:A:20:THR:HG23	1:A:28:ALA:HB1	1.94	0.50
1:A:158:ARG:HG3	1:A:205:LEU:HD23	1.95	0.49
1:A:43:ALA:HB2	1:A:83:LEU:HD13	1.95	0.49
1:B:2:VAL:HG23	1:B:3:GLN:H	1.77	0.48
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.49	0.48
1:B:107:ASP:HB3	1:B:110:ILE:HD12	1.96	0.47
1:B:20:THR:HG23	1:B:28:ALA:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LEU:HD22	1:B:309:LYS:HG3	1.96	0.47
1:B:328:ASP:HA	1:B:329:PRO:HD3	1.76	0.47
1:B:35:PRO:O	1:B:39:VAL:HG23	2.15	0.46
1:A:184:ASN:HD22	1:A:185:GLU:HB2	1.81	0.45
1:A:41:LYS:O	1:A:45:LEU:HG	2.16	0.45
1:A:317:LEU:O	1:A:321:ARG:HD2	2.17	0.45
1:A:328:ASP:HA	1:A:329:PRO:HD3	1.82	0.45
1:B:221:GLN:HE21	1:B:248:GLN:HB3	1.81	0.45
1:B:226:ASN:HB3	1:B:229:HIS:HB2	2.00	0.44
1:B:41:LYS:HG2	1:B:305:TRP:CD2	2.52	0.44
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.99	0.43
1:A:294:LYS:NZ	4:A:464(A):HOH:O	2.46	0.43
1:A:135:MET:HE3	1:A:177:ILE:HD13	2.01	0.42
1:B:55:ASN:HA	1:B:58:ILE:O	2.20	0.41
1:A:95:HIS:CD2	1:A:97:VAL:H	2.24	0.41
1:B:374:GLU:O	1:B:375:ARG:C	2.62	0.41
1:B:185:GLU:HA	1:B:186:PRO:HA	1.87	0.41
1:B:294:LYS:HA	1:B:295:PRO:HD3	1.94	0.41
1:A:249:ARG:O	1:A:252:LYS:HE3	2.21	0.41
1:A:35:PRO:O	1:A:39:VAL:HG23	2.21	0.40
1:A:180:GLU:HA	1:A:181:PRO:HD3	1.74	0.40
1:B:208:GLY:HA3	4:B:590(B):HOH:O	2.20	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LYS:NZ	1:B:276:ASN:O[6_665]	2.04	0.16
4:A:461(A):HOH:O	4:A:584(A):HOH:O[4_555]	2.17	0.03

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	391/394 (99%)	374 (96%)	16 (4%)	1 (0%)	36	55
1	B	391/394 (99%)	375 (96%)	13 (3%)	3 (1%)	16	31
All	All	782/788 (99%)	749 (96%)	29 (4%)	4 (0%)	24	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU
1	B	185	GLU
1	B	3	GLN
1	B	6	PRO

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	305/310 (98%)	287 (94%)	18 (6%)	18	37
1	B	305/310 (98%)	287 (94%)	18 (6%)	18	37
All	All	610/620 (98%)	574 (94%)	36 (6%)	18	37

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	50	ILE
1	A	68	GLU
1	A	69	LYS
1	A	83	LEU
1	A	149	ASP
1	A	150	LEU
1	A	174	ASN
1	A	184	ASN
1	A	213	LEU
1	A	273	LEU
1	A	284	LYS

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Mol	Chain	Res	Type
1	A	286	THR
1	A	302	ASP
1	A	359	ASN
1	A	361	SER
1	A	370	GLU
1	A	391	LEU
1	B	6	PRO
1	B	20	THR
1	B	41	LYS
1	B	58	ILE
1	B	61	ASP
1	B	66	GLU
1	B	69	LYS
1	B	90	THR
1	B	94	SER
1	B	131	GLU
1	B	149	ASP
1	B	235	LEU
1	B	273	LEU
1	B	286	THR
1	B	329	PRO
1	B	357	LEU
1	B	359	ASN
1	B	370	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	184	ASN
1	A	221	GLN
1	A	359	ASN
1	B	95	HIS
1	B	221	GLN
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 [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	B	400	3	9,9,9	1.18	1 (11%)	11,11,11	2.22	5 (45%)
2	XYL	A	400	3	9,9,9	0.81	0	11,11,11	1.78	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	B	400	3	-	1/12/12/12	-
2	XYL	A	400	3	-	1/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	XYL	C4-C3	-3.11	1.48	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	XYL	O5-C5-C4	-3.80	103.17	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	XYL	C1-C2-C3	-3.24	105.57	112.17
2	B	400	XYL	O1-C1-C2	3.06	117.58	111.16
2	A	400	XYL	O3-C3-C2	2.93	115.59	108.93
2	A	400	XYL	C5-C4-C3	2.78	117.84	112.17
2	B	400	XYL	O2-C2-C3	2.41	114.89	109.25
2	A	400	XYL	O2-C2-C1	-2.20	104.03	109.03
2	B	400	XYL	O3-C3-C4	2.17	113.87	108.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	400	XYL	O2-C2-C3-C4
2	A	400	XYL	O2-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.