



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:51 PM UTC

PDB ID : 1XLE / pdb_00001xle
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
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

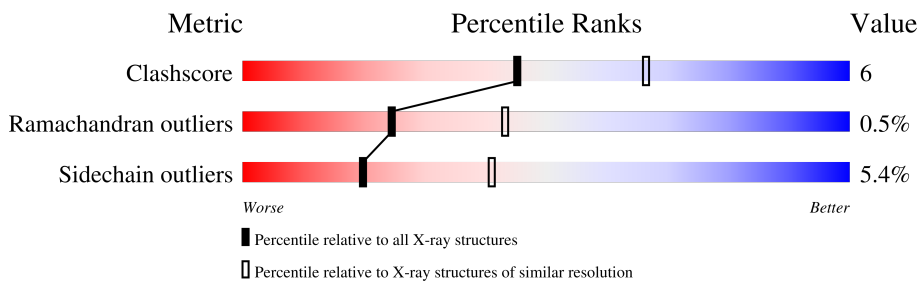
1 Overall quality at a glance

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	 43% 46% 9% •
1	B	394	 47% 45% 7% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6580 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 MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

- Molecule 3 is water.

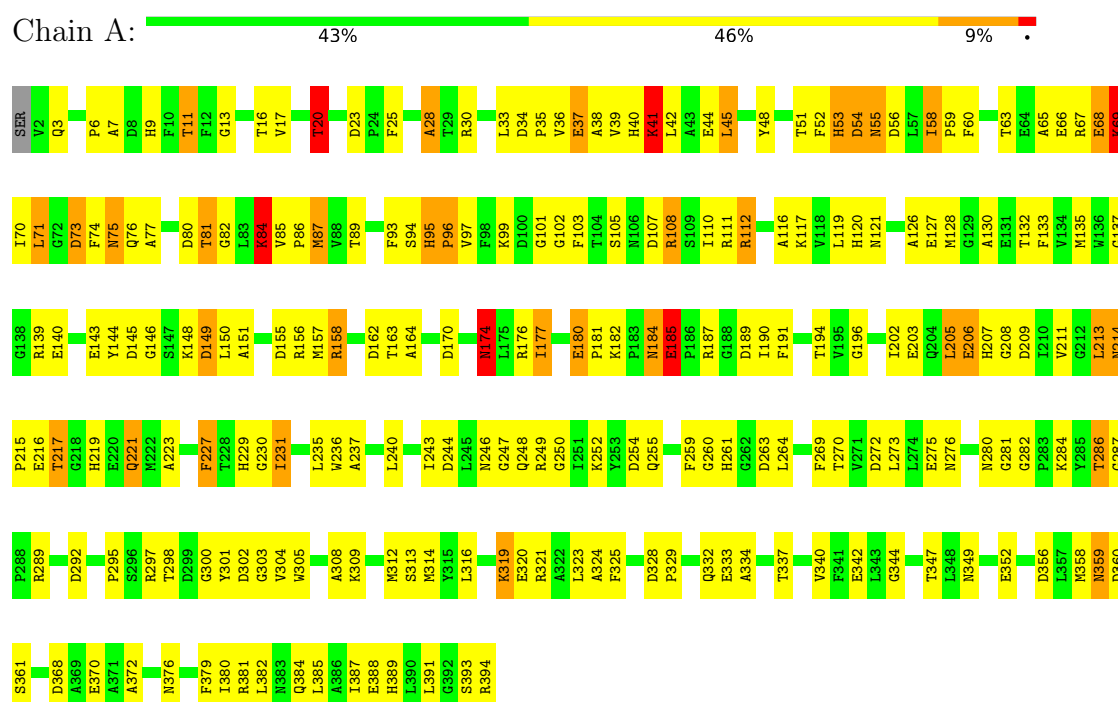
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	260	Total	O	0	0
			260	260		
3	B	262	Total	O	0	0
			262	262		

3 Residue-property plots

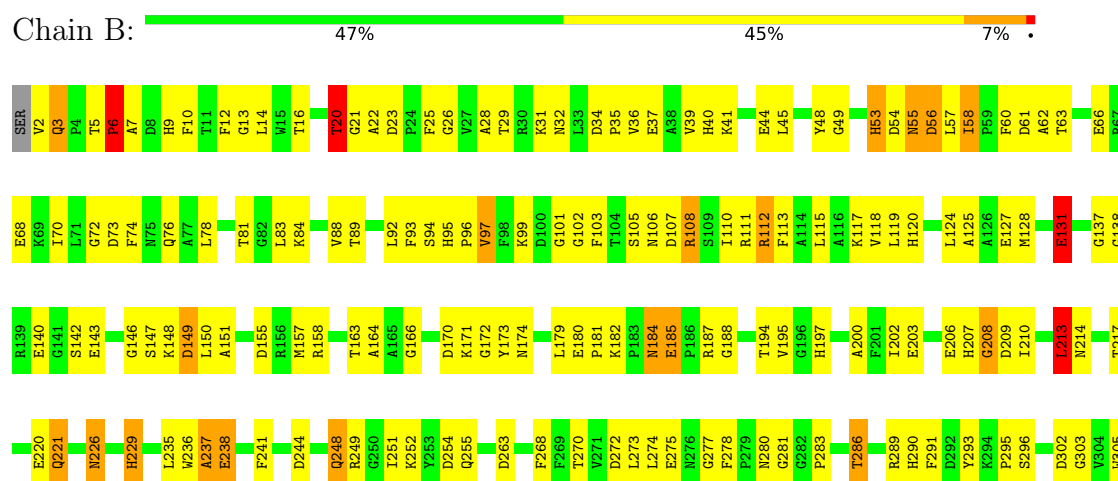
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

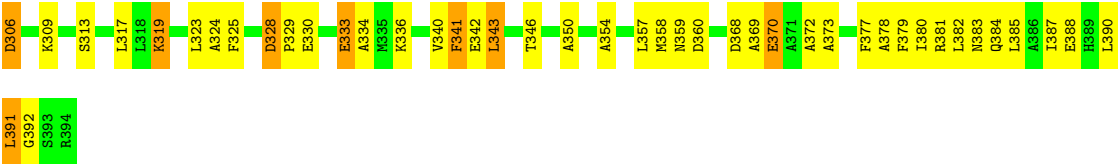
Note EDS was not executed.

• 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	105.40 Å 105.40 Å 154.00 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}	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6580	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: MN

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	1.48	14/3101 (0.5%)	2.84	328/4204 (7.8%)
1	B	1.50	14/3101 (0.5%)	2.76	278/4204 (6.6%)
All	All	1.49	28/6202 (0.5%)	2.80	606/8408 (7.2%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	ARG	CD-NE	-10.86	1.31	1.46
1	A	264	LEU	C-O	6.79	1.31	1.24
1	B	263	ASP	C-O	6.64	1.32	1.23
1	A	110	ILE	CA-CB	6.25	1.61	1.54
1	B	112	ARG	CD-NE	-6.19	1.37	1.46
1	B	53	HIS	CA-C	6.02	1.60	1.52
1	B	277	GLY	N-CA	5.99	1.54	1.45
1	A	337	THR	CA-CB	5.86	1.62	1.53
1	A	112	ARG	NE-CZ	-5.77	1.26	1.33
1	B	81	THR	CA-CB	5.67	1.62	1.53
1	A	103	PHE	C-O	5.65	1.30	1.24
1	B	20	THR	C-O	5.63	1.31	1.24
1	A	102	GLY	N-CA	5.62	1.53	1.45
1	A	145	ASP	C-O	5.55	1.31	1.24
1	A	289	ARG	CD-NE	-5.49	1.38	1.46
1	A	11	THR	C-O	5.46	1.31	1.23
1	B	149	ASP	CA-CB	-5.39	1.46	1.53
1	B	251	ILE	CA-CB	5.34	1.59	1.53
1	A	229	HIS	C-O	5.30	1.30	1.24
1	B	9	HIS	ND1-CE1	5.17	1.37	1.32
1	A	155	ASP	C-O	5.16	1.30	1.24
1	B	88	VAL	C-O	5.16	1.29	1.24
1	B	93	PHE	C-O	5.12	1.29	1.24
1	B	286	THR	CA-CB	5.12	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	ARG	CG-CD	-5.10	1.37	1.52
1	B	373	ALA	C-O	5.08	1.30	1.24
1	A	289	ARG	NE-CZ	-5.08	1.27	1.33
1	B	49	GLY	C-O	5.03	1.28	1.23

All (606) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ARG	CD-NE-CZ	35.82	174.55	124.40
1	A	158	ARG	CD-NE-CZ	25.45	160.03	124.40
1	A	112	ARG	CD-NE-CZ	25.02	159.42	124.40
1	A	289	ARG	CD-NE-CZ	19.91	152.28	124.40
1	A	359	ASN	CA-CB-CG	19.19	131.79	112.60
1	A	73	ASP	CA-CB-CG	17.38	129.98	112.60
1	B	238	GLU	N-CA-CB	-15.69	88.06	111.91
1	B	359	ASN	CA-CB-CG	15.28	127.88	112.60
1	B	379	PHE	CA-CB-CG	15.10	128.90	113.80
1	A	127	GLU	N-CA-CB	15.00	132.18	110.12
1	B	358	MET	CA-C-N	14.54	146.58	121.14
1	B	358	MET	C-N-CA	14.54	146.58	121.14
1	B	73	ASP	CA-CB-CG	14.33	126.93	112.60
1	A	394	ARG	CD-NE-CZ	13.84	143.77	124.40
1	A	379	PHE	CA-CB-CG	13.05	126.85	113.80
1	B	254	ASP	CA-CB-CG	12.91	125.51	112.60
1	A	158	ARG	CG-CD-NE	12.20	138.84	112.00
1	A	243	ILE	CA-C-O	-11.98	108.86	121.19
1	B	112	ARG	NE-CZ-NH2	11.83	129.85	119.20
1	B	238	GLU	CB-CA-C	11.77	127.64	111.86
1	A	107	ASP	CA-CB-CG	11.58	124.18	112.60
1	A	127	GLU	CB-CA-C	-11.19	92.22	110.79
1	B	55	ASN	CA-C-N	10.40	134.22	120.28
1	B	55	ASN	C-N-CA	10.40	134.22	120.28
1	A	28	ALA	CA-C-O	-10.31	109.81	121.15
1	B	101	GLY	O-C-N	10.30	133.13	123.35
1	B	255	GLN	OE1-CD-NE2	10.21	132.81	122.60
1	B	146	GLY	CA-C-N	9.97	134.63	120.28
1	B	146	GLY	C-N-CA	9.97	134.63	120.28
1	B	20	THR	N-CA-CB	-9.91	93.77	110.41
1	B	350	ALA	O-C-N	-9.88	110.63	122.89
1	B	324	ALA	CA-C-N	9.74	133.10	120.44
1	B	324	ALA	C-N-CA	9.74	133.10	120.44
1	B	392	GLY	CA-C-N	9.61	133.93	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	392	GLY	C-N-CA	9.61	133.93	120.29
1	B	20	THR	CA-CB-CG2	9.59	126.81	110.50
1	A	344	GLY	CA-C-N	9.54	135.55	121.72
1	A	344	GLY	C-N-CA	9.54	135.55	121.72
1	B	343	LEU	CA-C-N	9.49	132.27	120.22
1	B	343	LEU	C-N-CA	9.49	132.27	120.22
1	A	237	ALA	CA-C-N	9.43	135.44	122.34
1	A	237	ALA	C-N-CA	9.43	135.44	122.34
1	A	358	MET	CA-C-N	9.30	136.48	120.58
1	A	358	MET	C-N-CA	9.30	136.48	120.58
1	B	20	THR	CB-CA-C	9.25	128.35	109.95
1	A	352	GLU	CA-C-O	-9.17	110.46	120.36
1	A	58	ILE	CA-C-O	9.07	125.82	119.20
1	A	324	ALA	CA-C-N	9.04	132.73	120.44
1	A	324	ALA	C-N-CA	9.04	132.73	120.44
1	B	53	HIS	N-CA-CB	9.01	125.32	110.63
1	B	207	HIS	CA-CB-CG	-9.01	104.79	113.80
1	B	372	ALA	O-C-N	-9.00	111.89	122.15
1	B	143	GLU	CA-C-O	8.96	129.53	119.41
1	B	334	ALA	CA-C-N	8.95	132.27	120.28
1	B	334	ALA	C-N-CA	8.95	132.27	120.28
1	A	385	LEU	CA-C-O	-8.90	111.47	120.82
1	B	360	ASP	CA-C-O	8.90	130.59	120.98
1	A	230	GLY	O-C-N	-8.89	113.64	122.18
1	B	106	ASN	CA-C-N	8.88	134.02	121.24
1	B	106	ASN	C-N-CA	8.88	134.02	121.24
1	B	2	VAL	CA-C-N	8.84	143.37	121.80
1	B	2	VAL	C-N-CA	8.84	143.37	121.80
1	B	60	PHE	CA-CB-CG	8.83	122.63	113.80
1	A	394	ARG	NE-CZ-NH1	8.76	130.26	121.50
1	A	334	ALA	CA-C-N	8.76	132.01	120.28
1	A	334	ALA	C-N-CA	8.76	132.01	120.28
1	A	243	ILE	O-C-N	8.69	132.56	123.00
1	A	80	ASP	CA-CB-CG	8.63	121.23	112.60
1	B	207	HIS	CA-C-N	8.61	130.98	120.13
1	B	207	HIS	C-N-CA	8.61	130.98	120.13
1	B	23	ASP	CB-CA-C	8.58	127.08	110.17
1	B	241	PHE	CA-CB-CG	8.56	122.36	113.80
1	A	342	GLU	N-CA-CB	8.56	123.40	110.22
1	A	96	PRO	O-C-N	-8.55	112.41	122.24
1	A	101	GLY	O-C-N	8.54	131.46	123.35
1	B	96	PRO	CA-C-N	8.47	133.86	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	PRO	C-N-CA	8.47	133.86	120.47
1	A	158	ARG	NE-CZ-NH2	-8.47	111.58	119.20
1	B	238	GLU	CG-CD-OE2	8.44	137.81	118.40
1	B	76	GLN	CA-C-N	8.41	131.55	120.28
1	B	76	GLN	C-N-CA	8.41	131.55	120.28
1	A	56	ASP	CA-CB-CG	8.40	121.00	112.60
1	B	319	LYS	CA-C-N	8.31	131.24	120.44
1	B	319	LYS	C-N-CA	8.31	131.24	120.44
1	A	162	ASP	CA-CB-CG	8.31	120.91	112.60
1	A	65	ALA	N-CA-C	-8.22	102.00	110.97
1	B	101	GLY	CA-C-O	-8.21	114.83	122.13
1	B	213	LEU	CA-C-N	8.20	131.87	122.85
1	B	213	LEU	C-N-CA	8.20	131.87	122.85
1	B	103	PHE	CA-CB-CG	8.16	121.96	113.80
1	A	249	ARG	CD-NE-CZ	8.15	135.80	124.40
1	B	286	THR	N-CA-CB	-8.13	97.91	110.92
1	B	120	HIS	CA-C-N	8.12	132.66	120.31
1	B	120	HIS	C-N-CA	8.12	132.66	120.31
1	B	391	LEU	CA-C-N	8.11	137.51	121.53
1	B	391	LEU	C-N-CA	8.11	137.51	121.53
1	A	221	GLN	CA-C-N	8.09	134.23	120.72
1	A	221	GLN	C-N-CA	8.09	134.23	120.72
1	A	300	GLY	CA-C-O	-8.06	114.22	122.28
1	A	394	ARG	NE-CZ-NH2	-8.04	111.97	119.20
1	A	272	ASP	CA-C-N	8.02	131.68	120.29
1	A	272	ASP	C-N-CA	8.02	131.68	120.29
1	A	342	GLU	CB-CA-C	-8.01	95.81	110.63
1	B	244	ASP	CA-CB-CG	8.00	120.60	112.60
1	A	214	ASN	CB-CG-ND2	7.97	128.36	116.40
1	A	292	ASP	CA-CB-CG	7.93	120.53	112.60
1	A	39	VAL	CA-C-N	7.89	131.17	120.44
1	A	39	VAL	C-N-CA	7.89	131.17	120.44
1	B	48	TYR	N-CA-CB	-7.82	99.06	110.47
1	A	227	PHE	CA-C-N	7.77	131.03	120.54
1	A	227	PHE	C-N-CA	7.77	131.03	120.54
1	A	59	PRO	CB-CA-C	7.75	121.31	111.39
1	A	6	PRO	CA-C-N	7.74	136.50	121.18
1	A	6	PRO	C-N-CA	7.74	136.50	121.18
1	B	99	LYS	CA-C-O	-7.68	111.42	120.10
1	A	189	ASP	CA-C-O	-7.68	110.83	120.28
1	A	329	PRO	CA-C-N	7.66	130.55	120.28
1	A	329	PRO	C-N-CA	7.66	130.55	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	ALA	CA-C-N	7.65	132.98	122.34
1	B	237	ALA	C-N-CA	7.65	132.98	122.34
1	B	16	THR	CA-C-O	7.65	128.92	120.89
1	B	172	GLY	O-C-N	7.65	129.53	122.57
1	B	7	ALA	CA-C-N	7.64	131.93	120.31
1	B	7	ALA	C-N-CA	7.64	131.93	120.31
1	B	111	ARG	CA-C-N	7.63	130.37	120.44
1	B	111	ARG	C-N-CA	7.63	130.37	120.44
1	A	52	PHE	CA-C-N	7.62	134.00	122.65
1	A	52	PHE	C-N-CA	7.62	134.00	122.65
1	A	95	HIS	CA-C-N	7.61	127.99	119.32
1	A	95	HIS	C-N-CA	7.61	127.99	119.32
1	A	196	GLY	CA-C-N	7.61	130.47	120.28
1	A	196	GLY	C-N-CA	7.61	130.47	120.28
1	A	38	ALA	CA-C-N	7.60	130.13	120.56
1	A	38	ALA	C-N-CA	7.60	130.13	120.56
1	A	51	THR	CA-CB-CG2	7.56	123.36	110.50
1	A	342	GLU	CA-CB-CG	7.55	129.20	114.10
1	A	263	ASP	CA-CB-CG	7.50	120.11	112.60
1	B	36	VAL	CA-C-N	7.49	130.32	120.28
1	B	36	VAL	C-N-CA	7.49	130.32	120.28
1	B	203	GLU	CG-CD-OE2	7.48	135.60	118.40
1	A	170	ASP	CA-CB-CG	-7.42	105.18	112.60
1	A	359	ASN	CA-C-O	-7.39	112.03	120.24
1	A	23	ASP	CB-CA-C	7.37	124.69	110.17
1	A	53	HIS	CB-CA-C	-7.35	97.14	109.48
1	A	261	HIS	CA-C-N	7.33	135.79	121.41
1	A	261	HIS	C-N-CA	7.33	135.79	121.41
1	A	60	PHE	CA-CB-CG	7.33	121.13	113.80
1	B	346	THR	CA-CB-OG1	-7.32	98.62	109.60
1	B	214	ASN	CB-CG-ND2	7.32	127.38	116.40
1	B	163	THR	CA-CB-OG1	-7.32	98.63	109.60
1	B	25	PHE	CA-CB-CG	-7.31	106.49	113.80
1	B	200	ALA	CA-C-N	7.26	130.35	120.54
1	B	200	ALA	C-N-CA	7.26	130.35	120.54
1	A	94	SER	CA-C-O	-7.26	112.18	120.24
1	B	173	TYR	N-CA-C	-7.26	99.73	110.48
1	A	320	GLU	CA-CB-CG	7.26	128.61	114.10
1	A	254	ASP	CA-CB-CG	7.25	119.86	112.60
1	B	44	GLU	CG-CD-OE1	-7.25	101.72	118.40
1	A	340	VAL	CA-C-O	-7.23	113.50	121.17
1	A	77	ALA	CA-C-N	7.20	129.80	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ALA	C-N-CA	7.20	129.80	120.44
1	A	216	GLU	CA-C-O	7.16	128.09	120.36
1	B	208	GLY	CA-C-N	7.14	129.85	120.28
1	B	208	GLY	C-N-CA	7.14	129.85	120.28
1	B	283	PRO	CB-CA-C	7.13	120.28	110.95
1	A	194	THR	CA-CB-CG2	7.10	122.56	110.50
1	B	217	THR	CA-C-N	7.09	127.85	119.98
1	B	217	THR	C-N-CA	7.09	127.85	119.98
1	A	101	GLY	CA-C-O	-7.08	115.83	122.13
1	A	207	HIS	O-C-N	-7.07	112.43	121.97
1	A	63	THR	CA-C-N	7.07	129.75	120.28
1	A	63	THR	C-N-CA	7.07	129.75	120.28
1	A	250	GLY	N-CA-C	7.06	120.87	112.33
1	B	149	ASP	N-CA-C	-7.05	96.15	108.20
1	B	174	ASN	CA-C-N	7.05	134.49	122.37
1	B	174	ASN	C-N-CA	7.05	134.49	122.37
1	B	236	TRP	N-CA-CB	7.03	120.46	110.12
1	A	213	LEU	CD1-CG-CD2	-7.03	95.33	110.80
1	B	138	GLY	CA-C-O	-7.01	112.82	120.40
1	A	276	ASN	CA-C-O	-7.00	110.85	119.18
1	B	93	PHE	CA-C-O	-6.97	110.53	118.47
1	A	259	PHE	CA-C-N	6.95	133.25	122.20
1	A	259	PHE	C-N-CA	6.95	133.25	122.20
1	A	76	GLN	OE1-CD-NE2	6.95	129.55	122.60
1	A	108	ARG	NE-CZ-NH1	6.95	128.45	121.50
1	A	35	PRO	CA-C-N	6.92	129.53	120.60
1	A	35	PRO	C-N-CA	6.92	129.53	120.60
1	B	293	TYR	CB-CG-CD2	-6.91	110.43	120.80
1	A	119	LEU	CA-C-N	6.87	129.81	120.54
1	A	119	LEU	C-N-CA	6.87	129.81	120.54
1	B	305	TRP	CA-C-N	6.84	129.74	120.44
1	B	305	TRP	C-N-CA	6.84	129.74	120.44
1	A	149	ASP	N-CA-C	-6.83	95.04	107.75
1	B	360	ASP	CA-C-N	6.79	131.01	120.82
1	B	360	ASP	C-N-CA	6.79	131.01	120.82
1	B	84	LYS	N-CA-C	-6.79	100.75	110.59
1	B	14	LEU	CA-C-O	6.77	127.75	119.97
1	B	197	HIS	CA-C-N	6.76	127.45	119.94
1	B	197	HIS	C-N-CA	6.76	127.45	119.94
1	B	149	ASP	CA-CB-CG	6.75	119.35	112.60
1	A	81	THR	CA-CB-OG1	-6.75	99.48	109.60
1	B	226	ASN	CA-CB-CG	-6.71	105.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	PHE	CA-CB-CG	6.70	120.50	113.80
1	A	344	GLY	N-CA-C	6.68	122.02	114.67
1	B	97	VAL	CA-CB-CG1	6.67	121.74	110.40
1	A	356	ASP	CA-C-N	6.67	129.50	120.44
1	A	356	ASP	C-N-CA	6.67	129.50	120.44
1	A	144	TYR	CA-C-O	6.66	127.90	120.70
1	B	164	ALA	CA-C-N	6.66	129.10	120.44
1	B	164	ALA	C-N-CA	6.66	129.10	120.44
1	B	383	ASN	CA-C-N	6.66	129.50	120.38
1	B	383	ASN	C-N-CA	6.66	129.50	120.38
1	A	117	LYS	CA-C-N	6.65	129.07	120.56
1	A	117	LYS	C-N-CA	6.65	129.07	120.56
1	A	130	ALA	CA-C-O	-6.63	113.74	121.16
1	A	260	GLY	CA-C-N	6.62	133.94	122.56
1	A	260	GLY	C-N-CA	6.62	133.94	122.56
1	A	295	PRO	CA-C-O	-6.60	114.17	121.23
1	A	66	GLU	O-C-N	-6.59	115.23	122.09
1	A	34	ASP	CA-CB-CG	6.59	119.19	112.60
1	A	6	PRO	O-C-N	-6.58	113.75	122.64
1	A	94	SER	N-CA-C	6.58	119.78	111.69
1	B	53	HIS	N-CA-C	-6.57	99.60	110.17
1	B	187	ARG	NE-CZ-NH1	6.55	128.05	121.50
1	A	20	THR	CB-CA-C	6.53	122.95	109.95
1	A	133	PHE	CA-CB-CG	-6.52	107.28	113.80
1	A	51	THR	CA-CB-OG1	-6.52	99.82	109.60
1	A	48	TYR	N-CA-C	-6.51	102.66	112.04
1	A	217	THR	CA-C-N	6.50	128.48	120.22
1	A	217	THR	C-N-CA	6.50	128.48	120.22
1	B	102	GLY	CA-C-N	6.50	129.87	120.38
1	B	102	GLY	C-N-CA	6.50	129.87	120.38
1	B	163	THR	CA-C-O	-6.49	114.01	120.70
1	B	127	GLU	CA-CB-CG	6.48	127.07	114.10
1	A	209	ASP	CA-CB-CG	6.48	119.08	112.60
1	B	354	ALA	N-CA-C	-6.47	104.15	111.07
1	A	120	HIS	O-C-N	-6.46	115.37	122.09
1	B	92	LEU	CA-C-O	6.41	128.54	120.65
1	B	155	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	76	GLN	CA-C-N	6.39	129.17	120.54
1	A	76	GLN	C-N-CA	6.39	129.17	120.54
1	A	75	ASN	CA-C-N	6.38	129.08	120.65
1	A	75	ASN	C-N-CA	6.38	129.08	120.65
1	A	223	ALA	CA-C-N	6.38	131.87	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	ALA	C-N-CA	6.38	131.87	120.77
1	A	312	MET	CA-C-N	6.37	128.72	120.44
1	A	312	MET	C-N-CA	6.37	128.72	120.44
1	A	325	PHE	CA-CB-CG	6.37	120.17	113.80
1	A	321	ARG	CA-C-N	6.36	129.98	120.31
1	A	321	ARG	C-N-CA	6.36	129.98	120.31
1	B	78	LEU	N-CA-C	-6.36	104.27	111.07
1	B	325	PHE	CA-CB-CG	6.35	120.15	113.80
1	A	149	ASP	N-CA-CB	6.34	120.86	110.39
1	B	60	PHE	CA-C-N	6.34	132.24	121.14
1	B	60	PHE	C-N-CA	6.34	132.24	121.14
1	B	333	GLU	CA-C-N	6.33	128.77	120.28
1	B	333	GLU	C-N-CA	6.33	128.77	120.28
1	A	214	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	B	194	THR	CA-CB-CG2	6.32	121.24	110.50
1	A	359	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	A	180	GLU	CG-CD-OE1	6.31	132.92	118.40
1	B	110	ILE	CB-CG1-CD1	6.31	127.06	113.80
1	A	82	GLY	CA-C-N	6.30	129.65	120.71
1	A	82	GLY	C-N-CA	6.30	129.65	120.71
1	A	347	THR	CA-CB-OG1	-6.29	100.16	109.60
1	A	356	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	66	GLU	CA-C-N	6.28	129.02	120.54
1	A	66	GLU	C-N-CA	6.28	129.02	120.54
1	B	236	TRP	CA-C-O	-6.28	113.89	120.55
1	A	302	ASP	CA-C-N	6.26	127.05	120.03
1	A	302	ASP	C-N-CA	6.26	127.05	120.03
1	A	211	VAL	CA-CB-CG2	6.25	121.03	110.40
1	A	370	GLU	CB-CG-CD	6.25	123.22	112.60
1	A	102	GLY	N-CA-C	-6.23	98.41	113.18
1	A	20	THR	CA-CB-CG2	6.22	121.08	110.50
1	B	350	ALA	CA-C-N	-6.20	113.80	122.86
1	B	350	ALA	C-N-CA	-6.20	113.80	122.86
1	A	381	ARG	NE-CZ-NH1	6.20	127.70	121.50
1	A	54	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	370	GLU	CA-C-O	-6.19	113.99	120.55
1	B	150	LEU	CB-CA-C	6.18	121.05	110.79
1	B	32	ASN	CA-CB-CG	-6.18	106.42	112.60
1	A	127	GLU	CG-CD-OE1	6.18	132.61	118.40
1	A	70	ILE	O-C-N	6.17	128.12	121.94
1	A	264	LEU	CB-CA-C	6.17	120.52	110.95
1	B	302	ASP	CA-C-N	6.17	128.12	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	ASP	C-N-CA	6.17	128.12	120.34
1	B	22	ALA	CB-CA-C	6.17	119.90	109.84
1	B	58	ILE	O-C-N	6.17	126.86	121.12
1	A	389	HIS	CA-CB-CG	-6.16	107.64	113.80
1	A	244	ASP	CA-CB-CG	6.15	118.75	112.60
1	B	214	ASN	CA-CB-CG	6.14	118.74	112.60
1	B	354	ALA	N-CA-CB	6.13	118.91	110.01
1	A	255	GLN	OE1-CD-NE2	6.13	128.73	122.60
1	A	127	GLU	CB-CG-CD	6.13	123.02	112.60
1	A	56	ASP	N-CA-C	-6.12	104.69	111.36
1	A	69	LYS	CA-C-O	6.10	127.41	121.00
1	A	143	GLU	CA-C-O	6.10	126.31	119.41
1	A	87	MET	CA-C-N	6.10	132.38	122.69
1	A	87	MET	C-N-CA	6.10	132.38	122.69
1	A	17	VAL	CA-C-O	-6.09	113.89	120.47
1	A	372	ALA	O-C-N	-6.09	114.77	122.27
1	A	213	LEU	CA-C-N	6.09	129.55	122.85
1	A	213	LEU	C-N-CA	6.09	129.55	122.85
1	A	309	LYS	CA-C-N	6.08	128.43	120.28
1	A	309	LYS	C-N-CA	6.08	128.43	120.28
1	A	87	MET	CA-CB-CG	6.08	126.26	114.10
1	B	213	LEU	CA-CB-CG	6.08	137.57	116.30
1	B	131	GLU	CB-CG-CD	6.06	122.91	112.60
1	A	254	ASP	CB-CA-C	6.06	120.57	110.88
1	B	236	TRP	CA-CB-CG	6.05	125.10	113.60
1	B	248	GLN	CA-C-N	-6.05	113.81	122.77
1	B	248	GLN	C-N-CA	-6.05	113.81	122.77
1	B	313	SER	CA-C-N	6.05	128.71	120.54
1	B	313	SER	C-N-CA	6.05	128.71	120.54
1	A	137	GLY	CA-C-N	6.04	133.92	121.17
1	A	137	GLY	C-N-CA	6.04	133.92	121.17
1	A	75	ASN	CA-CB-CG	6.02	118.62	112.60
1	A	38	ALA	O-C-N	6.02	128.59	122.09
1	A	368	ASP	CB-CG-OD2	6.02	132.24	118.40
1	B	368	ASP	CA-CB-CG	6.01	118.61	112.60
1	B	229	HIS	CA-C-N	6.01	126.61	119.94
1	B	229	HIS	C-N-CA	6.01	126.61	119.94
1	A	227	PHE	CA-C-O	6.00	127.31	120.90
1	A	298	THR	CA-C-N	5.99	130.96	122.09
1	A	298	THR	C-N-CA	5.99	130.96	122.09
1	B	369	ALA	CA-C-O	5.99	126.87	120.70
1	A	384	GLN	N-CA-C	-5.97	104.69	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	GLN	O-C-N	5.96	128.18	121.32
1	B	37	GLU	CA-C-N	5.96	128.18	120.44
1	B	37	GLU	C-N-CA	5.96	128.18	120.44
1	B	166	GLY	CA-C-O	-5.95	114.62	120.75
1	A	280	ASN	OD1-CG-ND2	-5.95	116.65	122.60
1	B	40	HIS	CA-C-O	-5.94	114.59	120.82
1	A	74	PHE	CA-CB-CG	5.93	119.73	113.80
1	A	108	ARG	CA-C-O	-5.93	114.13	120.42
1	B	29	THR	CA-CB-OG1	-5.88	100.77	109.60
1	B	26	GLY	N-CA-C	5.88	119.67	110.91
1	A	388	GLU	CA-C-O	-5.87	114.33	120.55
1	B	382	LEU	CA-C-O	-5.87	113.46	120.10
1	A	128	MET	O-C-N	-5.87	114.36	122.46
1	A	319	LYS	CA-C-N	5.86	128.06	120.44
1	A	319	LYS	C-N-CA	5.86	128.06	120.44
1	B	148	LYS	N-CA-C	5.86	118.76	109.50
1	B	388	GLU	CA-C-N	5.86	128.61	120.29
1	B	388	GLU	C-N-CA	5.86	128.61	120.29
1	A	349	ASN	CB-CG-ND2	5.86	125.18	116.40
1	B	16	THR	CB-CA-C	5.86	120.70	111.39
1	B	342	GLU	CG-CD-OE2	-5.85	104.95	118.40
1	A	110	ILE	O-C-N	-5.85	116.09	121.94
1	A	66	GLU	CB-CG-CD	5.84	122.52	112.60
1	B	188	GLY	N-CA-C	-5.83	105.73	112.50
1	A	332	GLN	CA-C-O	-5.83	114.37	120.55
1	B	278	PHE	N-CA-C	5.83	118.35	110.31
1	B	384	GLN	CA-C-N	5.82	128.56	120.29
1	B	384	GLN	C-N-CA	5.82	128.56	120.29
1	B	210	ILE	CA-C-N	5.82	130.40	123.19
1	B	210	ILE	C-N-CA	5.82	130.40	123.19
1	B	209	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	137	GLY	CA-C-N	5.80	127.40	120.14
1	B	137	GLY	C-N-CA	5.80	127.40	120.14
1	B	274	LEU	CA-C-O	-5.80	114.27	120.42
1	A	205	LEU	CA-C-O	5.80	127.66	121.05
1	B	203	GLU	CA-C-N	5.80	131.48	122.49
1	B	203	GLU	C-N-CA	5.80	131.48	122.49
1	A	320	GLU	CA-C-N	5.79	128.04	120.28
1	A	320	GLU	C-N-CA	5.79	128.04	120.28
1	A	174	ASN	CA-C-N	5.78	132.30	122.37
1	A	174	ASN	C-N-CA	5.78	132.30	122.37
1	A	70	ILE	CA-C-O	-5.77	115.27	121.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	ARG	NE-CZ-NH2	-5.77	114.01	119.20
1	A	105	SER	CA-C-N	5.77	130.49	120.68
1	A	105	SER	C-N-CA	5.77	130.49	120.68
1	B	107	ASP	CA-CB-CG	-5.77	106.83	112.60
1	B	112	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	A	42	LEU	CA-C-N	5.76	127.92	120.44
1	A	42	LEU	C-N-CA	5.76	127.92	120.44
1	B	270	THR	N-CA-C	-5.75	104.93	111.14
1	A	352	GLU	N-CA-C	-5.75	99.53	108.90
1	B	37	GLU	CB-CG-CD	5.75	122.38	112.60
1	B	359	ASN	CB-CA-C	5.75	122.00	109.99
1	B	166	GLY	N-CA-C	-5.74	105.84	112.73
1	B	182	LYS	O-C-N	5.74	127.92	121.32
1	B	56	ASP	N-CA-CB	5.73	118.55	110.12
1	A	7	ALA	CA-C-N	5.73	131.16	121.14
1	A	7	ALA	C-N-CA	5.73	131.16	121.14
1	B	97	VAL	CA-C-O	-5.73	114.44	120.57
1	A	60	PHE	CA-C-N	5.72	132.39	122.56
1	A	60	PHE	C-N-CA	5.72	132.39	122.56
1	B	151	ALA	O-C-N	-5.71	116.18	122.07
1	A	139	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	A	303	GLY	O-C-N	-5.71	116.63	122.17
1	A	45	LEU	CA-C-O	-5.71	113.06	119.79
1	B	207	HIS	O-C-N	-5.70	114.83	122.19
1	A	185	GLU	CB-CG-CD	5.70	122.29	112.60
1	B	57	LEU	CB-CA-C	5.69	119.74	110.24
1	A	41	LYS	N-CA-C	5.68	117.47	111.28
1	A	96	PRO	CA-C-N	5.68	128.54	120.53
1	A	96	PRO	C-N-CA	5.68	128.54	120.53
1	A	349	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	B	286	THR	CB-CA-C	5.67	120.15	111.02
1	A	25	PHE	CA-CB-CG	-5.66	108.14	113.80
1	B	360	ASP	O-C-N	-5.65	115.00	122.57
1	A	361	SER	N-CA-C	5.65	117.44	111.28
1	B	72	GLY	O-C-N	5.64	127.60	122.19
1	A	352	GLU	O-C-N	5.63	130.01	123.30
1	A	151	ALA	N-CA-C	-5.63	105.23	111.36
1	B	330	GLU	CA-C-N	5.62	128.41	120.42
1	B	330	GLU	C-N-CA	5.62	128.41	120.42
1	B	379	PHE	CB-CA-C	5.62	121.84	110.38
1	B	120	HIS	CA-CB-CG	-5.61	108.19	113.80
1	A	286	THR	CA-C-O	-5.60	112.89	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ASN	O-C-N	5.60	129.24	122.75
1	A	391	LEU	CA-C-N	5.60	132.38	121.41
1	A	391	LEU	C-N-CA	5.60	132.38	121.41
1	A	37	GLU	CB-CG-CD	5.59	122.11	112.60
1	A	244	ASP	CA-C-O	-5.59	114.53	120.40
1	B	74	PHE	N-CA-CB	5.59	118.12	110.01
1	B	380	ILE	N-CA-C	-5.59	105.28	110.53
1	B	142	SER	CA-C-O	-5.58	115.26	121.23
1	B	295	PRO	CA-C-O	-5.58	115.26	121.23
1	A	221	GLN	O-C-N	-5.57	114.77	122.46
1	B	12	PHE	CA-C-O	-5.57	114.25	120.66
1	A	297	ARG	CG-CD-NE	5.57	124.24	112.00
1	B	358	MET	CA-C-O	5.56	126.66	120.82
1	A	187	ARG	NE-CZ-NH2	-5.55	114.20	119.20
1	A	55	ASN	N-CA-C	5.55	119.80	113.19
1	B	34	ASP	CA-C-N	5.55	125.21	119.05
1	B	34	ASP	C-N-CA	5.55	125.21	119.05
1	B	118	VAL	O-C-N	5.55	127.67	121.90
1	B	147	SER	CA-C-N	5.55	131.27	122.62
1	B	147	SER	C-N-CA	5.55	131.27	122.62
1	A	33	LEU	CA-C-O	-5.54	114.28	120.54
1	B	171	LYS	CA-C-O	5.54	126.18	119.31
1	A	259	PHE	CA-C-O	5.53	126.99	120.96
1	A	56	ASP	N-CA-CB	5.53	118.34	110.16
1	B	340	VAL	O-C-N	-5.52	116.51	121.87
1	B	185	GLU	CA-CB-CG	5.52	125.15	114.10
1	A	177	ILE	O-C-N	5.51	129.22	122.83
1	A	387	ILE	CA-C-N	5.51	127.66	120.28
1	A	387	ILE	C-N-CA	5.51	127.66	120.28
1	A	368	ASP	OD1-CG-OD2	-5.50	109.70	122.90
1	B	340	VAL	CB-CA-C	5.50	119.56	112.14
1	A	236	TRP	O-C-N	-5.49	116.30	122.12
1	A	333	GLU	CA-C-N	5.49	127.90	120.38
1	A	333	GLU	C-N-CA	5.49	127.90	120.38
1	A	270	THR	CA-CB-OG1	-5.49	101.37	109.60
1	A	202	ILE	CA-C-O	-5.48	115.35	121.05
1	B	281	GLY	CA-C-O	-5.47	117.86	122.29
1	A	3	GLN	CA-C-O	5.47	123.86	119.59
1	A	156	ARG	CD-NE-CZ	5.46	132.05	124.40
1	A	163	THR	CA-C-N	5.46	128.05	120.29
1	A	163	THR	C-N-CA	5.46	128.05	120.29
1	B	370	GLU	CA-C-O	-5.46	114.73	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	GLU	CG-CD-OE2	5.45	130.94	118.40
1	A	360	ASP	CA-C-N	5.45	127.58	120.28
1	A	360	ASP	C-N-CA	5.45	127.58	120.28
1	A	295	PRO	N-CA-C	-5.45	102.64	111.03
1	B	92	LEU	O-C-N	-5.45	114.90	122.20
1	A	370	GLU	CG-CD-OE2	5.44	130.91	118.40
1	A	320	GLU	CG-CD-OE2	5.43	130.90	118.40
1	B	54	ASP	O-C-N	-5.43	116.44	122.09
1	A	164	ALA	CA-C-N	5.43	128.00	120.29
1	A	164	ALA	C-N-CA	5.43	128.00	120.29
1	B	372	ALA	CB-CA-C	5.43	120.07	110.85
1	B	108	ARG	NE-CZ-NH2	-5.42	114.32	119.20
1	A	158	ARG	CA-C-O	5.41	126.69	120.90
1	A	16	THR	O-C-N	-5.41	115.40	122.59
1	B	255	GLN	CB-CG-CD	-5.39	103.44	112.60
1	B	63	THR	CA-CB-OG1	-5.39	101.52	109.60
1	A	139	ARG	NH1-CZ-NH2	-5.38	112.30	119.30
1	B	206	GLU	N-CA-C	-5.38	104.84	111.40
1	B	330	GLU	CA-C-O	-5.38	114.72	120.42
1	A	247	GLY	CA-C-O	5.38	126.31	121.47
1	A	368	ASP	CA-C-N	5.37	127.43	120.44
1	A	368	ASP	C-N-CA	5.37	127.43	120.44
1	B	290	HIS	CA-CB-CG	5.37	119.17	113.80
1	B	317	LEU	CA-C-O	-5.37	115.18	120.82
1	B	255	GLN	CG-CD-OE1	-5.37	110.06	120.80
1	B	108	ARG	NE-CZ-NH1	5.37	126.87	121.50
1	B	143	GLU	CA-C-N	5.37	130.99	122.94
1	B	143	GLU	C-N-CA	5.37	130.99	122.94
1	B	323	LEU	N-CA-CB	5.37	118.19	110.20
1	A	316	LEU	CA-C-N	5.36	127.46	120.28
1	A	316	LEU	C-N-CA	5.36	127.46	120.28
1	B	252	LYS	CA-CB-CG	5.36	124.81	114.10
1	A	382	LEU	CA-C-N	5.36	127.89	120.29
1	A	382	LEU	C-N-CA	5.36	127.89	120.29
1	B	286	THR	OG1-CB-CG2	5.35	119.99	109.30
1	A	99	LYS	N-CA-C	5.34	118.90	112.38
1	B	44	GLU	CG-CD-OE2	5.34	130.69	118.40
1	A	328	ASP	CA-C-N	5.34	125.41	119.32
1	A	328	ASP	C-N-CA	5.34	125.41	119.32
1	A	146	GLY	CA-C-N	5.34	129.64	120.72
1	A	146	GLY	C-N-CA	5.34	129.64	120.72
1	A	170	ASP	N-CA-C	5.34	117.79	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	ASP	O-C-N	-5.34	116.46	122.12
1	B	119	LEU	CA-C-N	5.34	127.97	120.28
1	B	119	LEU	C-N-CA	5.34	127.97	120.28
1	B	179	LEU	CA-C-O	5.34	127.06	120.92
1	A	320	GLU	CB-CG-CD	5.33	121.67	112.60
1	A	252	LYS	CA-C-N	5.33	129.87	120.87
1	A	252	LYS	C-N-CA	5.33	129.87	120.87
1	B	13	GLY	CA-C-N	5.33	128.41	120.31
1	B	13	GLY	C-N-CA	5.33	128.41	120.31
1	A	190	ILE	O-C-N	5.32	128.57	123.14
1	A	71	LEU	CA-C-N	5.32	126.97	120.22
1	A	71	LEU	C-N-CA	5.32	126.97	120.22
1	A	376	ASN	N-CA-CB	5.32	118.27	110.35
1	B	289	ARG	CD-NE-CZ	5.32	131.84	124.40
1	B	113	PHE	N-CA-CB	5.30	117.70	110.01
1	B	55	ASN	O-C-N	-5.30	115.14	122.46
1	B	385	LEU	CA-C-O	-5.30	114.80	120.42
1	A	273	LEU	CA-C-O	-5.30	114.81	120.42
1	B	202	ILE	CA-C-N	5.29	131.66	121.18
1	B	202	ILE	C-N-CA	5.29	131.66	121.18
1	B	6	PRO	O-C-N	-5.29	115.49	122.64
1	A	176	ARG	NH1-CZ-NH2	-5.29	112.42	119.30
1	A	203	GLU	N-CA-C	5.29	119.22	112.87
1	B	249	ARG	O-C-N	-5.29	116.18	122.63
1	B	70	ILE	CA-C-N	5.28	127.89	120.28
1	B	70	ILE	C-N-CA	5.28	127.89	120.28
1	A	128	MET	CA-C-N	5.28	131.93	121.53
1	A	128	MET	C-N-CA	5.28	131.93	121.53
1	A	213	LEU	N-CA-CB	-5.28	102.72	110.85
1	A	287	GLY	CA-C-O	5.28	129.07	121.52
1	A	316	LEU	CB-CA-C	5.28	119.55	110.79
1	A	393	SER	CA-C-N	5.28	131.19	121.70
1	A	393	SER	C-N-CA	5.28	131.19	121.70
1	A	301	TYR	CA-C-O	-5.27	114.15	120.10
1	B	125	ALA	CA-C-N	5.27	127.29	120.44
1	B	125	ALA	C-N-CA	5.27	127.29	120.44
1	B	291	PHE	CA-C-O	5.27	126.12	120.32
1	B	248	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	A	111	ARG	CA-CB-CG	5.25	124.61	114.10
1	A	347	THR	CA-CB-CG2	5.25	119.43	110.50
1	B	238	GLU	CB-CG-CD	5.25	121.53	112.60
1	A	387	ILE	O-C-N	-5.25	116.78	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	340	VAL	O-C-N	5.23	127.04	121.91
1	B	317	LEU	O-C-N	5.23	127.46	122.07
1	B	274	LEU	O-C-N	5.23	128.11	122.15
1	A	208	GLY	CA-C-N	5.23	127.29	120.28
1	A	208	GLY	C-N-CA	5.23	127.29	120.28
1	A	126	ALA	O-C-N	-5.22	116.45	122.09
1	B	23	ASP	O-C-N	-5.22	115.31	121.32
1	A	303	GLY	CA-C-N	5.20	127.11	120.56
1	A	303	GLY	C-N-CA	5.20	127.11	120.56
1	A	305	TRP	CA-C-N	5.19	127.50	120.65
1	A	305	TRP	C-N-CA	5.19	127.50	120.65
1	A	269	PHE	CA-C-O	-5.19	114.00	119.97
1	B	10	PHE	CB-CA-C	5.19	119.44	110.77
1	A	93	PHE	CA-C-O	-5.19	112.56	118.47
1	A	349	ASN	N-CA-C	-5.18	102.39	110.42
1	B	68	GLU	CB-CA-C	5.18	119.66	110.85
1	B	381	ARG	N-CA-CB	5.18	117.52	110.01
1	B	221	GLN	CA-C-O	-5.18	113.23	119.49
1	A	13	GLY	N-CA-C	-5.17	104.80	113.02
1	A	67	ARG	CG-CD-NE	-5.16	100.64	112.00
1	B	5	THR	CA-C-N	5.16	126.29	119.84
1	B	5	THR	C-N-CA	5.16	126.29	119.84
1	A	30	ARG	O-C-N	5.16	129.58	123.24
1	A	323	LEU	N-CA-C	-5.15	105.74	112.23
1	B	21	GLY	CA-C-N	-5.15	114.13	121.50
1	B	21	GLY	C-N-CA	-5.15	114.13	121.50
1	A	372	ALA	CA-C-O	5.15	125.89	119.97
1	A	84	LYS	O-C-N	-5.15	116.66	122.68
1	B	83	LEU	CA-C-O	5.15	127.17	121.56
1	A	236	TRP	CA-C-N	5.14	131.60	121.58
1	A	236	TRP	C-N-CA	5.14	131.60	121.58
1	B	208	GLY	O-C-N	-5.13	116.90	122.19
1	A	121	ASN	CA-C-N	5.13	127.02	120.56
1	A	121	ASN	C-N-CA	5.13	127.02	120.56
1	A	281	GLY	CA-C-O	-5.13	117.26	122.59
1	B	328	ASP	CA-C-N	5.13	125.42	119.47
1	B	328	ASP	C-N-CA	5.13	125.42	119.47
1	B	31	LYS	CA-C-O	-5.12	115.58	121.47
1	A	187	ARG	N-CA-C	-5.12	103.16	110.59
1	A	119	LEU	CB-CA-C	5.11	119.05	110.92
1	B	55	ASN	CB-CA-C	5.11	120.59	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	THR	CA-CB-CG2	5.09	119.15	110.50
1	B	187	ARG	CD-NE-CZ	5.09	131.52	124.40
1	B	117	LYS	CA-C-N	5.08	127.07	120.56
1	B	117	LYS	C-N-CA	5.08	127.07	120.56
1	B	272	ASP	O-C-N	-5.08	116.84	122.07
1	A	304	VAL	CB-CA-C	5.08	118.47	111.97
1	B	334	ALA	N-CA-C	-5.08	105.75	111.28
1	A	379	PHE	N-CA-C	-5.07	105.84	112.23
1	A	216	GLU	O-C-N	-5.07	117.27	123.30
1	A	68	GLU	CA-CB-CG	-5.05	103.99	114.10
1	B	105	SER	N-CA-CB	5.05	117.46	109.83
1	A	116	ALA	CA-C-O	5.05	126.12	120.82
1	B	149	ASP	N-CA-CB	5.05	118.70	110.37
1	B	341	PHE	N-CA-C	-5.05	105.86	111.36
1	B	143	GLU	O-C-N	-5.04	115.19	122.36
1	A	308	ALA	CA-C-O	5.04	126.11	120.82
1	A	36	VAL	CA-C-N	5.04	127.53	120.28
1	A	36	VAL	C-N-CA	5.04	127.53	120.28
1	B	115	LEU	CB-CA-C	5.03	119.41	110.85
1	B	336	LYS	CA-C-N	5.03	126.98	120.44
1	B	336	LYS	C-N-CA	5.03	126.98	120.44
1	A	9	HIS	CA-CB-CG	-5.03	108.77	113.80
1	A	282	GLY	N-CA-C	-5.02	102.10	112.34
1	A	231	ILE	CA-C-N	5.01	127.00	120.28
1	A	231	ILE	C-N-CA	5.01	127.00	120.28
1	B	32	ASN	OD1-CG-ND2	5.01	127.61	122.60

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	2882	39	0
1	B	3027	0	2882	34	1
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
3	A	260	0	0	5	1
3	B	262	0	0	4	1
All	All	6580	0	5764	70	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 6.

All (70) 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:61:ASP:OD1	3:B:427(B):HOH:O	1.71	1.05
1:A:75:ASN:ND2	3:A:599(A):HOH:O	2.12	0.83
1:B:238:GLU:OE1	3:B:710(B):HOH:O	2.03	0.76
1:A:206:GLU:HG2	3:A:803(A):HOH:O	1.86	0.76
1:A:95:HIS:HD2	1:A:97:VAL:H	1.40	0.70
1:A:174:ASN:N	1:A:174:ASN:HD22	1.92	0.67
1:A:206:GLU:CG	3:A:803(A):HOH:O	2.45	0.63
1:B:95:HIS:HD2	1:B:97:VAL:H	1.45	0.62
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.84	0.60
1:A:158:ARG:HG3	1:A:205:LEU:HD23	1.86	0.57
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.89	0.55
1:A:184:ASN:HD22	1:A:185:GLU:HB2	1.72	0.55
1:B:61:ASP:OD1	1:B:61:ASP:C	2.49	0.55
1:B:140:GLU:HG3	1:B:157:MET:HE1	1.89	0.54
1:A:108:ARG:O	1:A:112:ARG:HG3	2.08	0.53
1:A:95:HIS:CD2	1:A:97:VAL:H	2.22	0.53
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.73	0.53
1:B:226:ASN:HB3	1:B:229:HIS:HB2	1.89	0.53
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.91	0.53
1:A:20:THR:HG23	1:A:28:ALA:CB	2.39	0.53
1:B:124:LEU:HD11	1:B:128:MET:HE2	1.93	0.51
1:A:275:GLU:HG3	1:A:319:LYS:HG3	1.93	0.51
1:B:45:LEU:HD22	1:B:309:LYS:HG2	1.93	0.50
1:A:20:THR:HG23	1:A:28:ALA:HB1	1.93	0.50
1:B:55:ASN:HA	1:B:58:ILE:O	2.12	0.49
1:A:41:LYS:O	1:A:45:LEU:HG	2.13	0.49
1:A:174:ASN:N	1:A:174:ASN:ND2	2.61	0.48
1:B:61:ASP:OD1	1:B:61:ASP:O	2.30	0.48
1:A:58:ILE:HD11	1:A:71:LEU:HG	1.96	0.47
1:A:135:MET:HE3	1:A:177:ILE:HG21	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:VAL:HG23	1:B:220:GLU:CD	2.40	0.47
1:B:237:ALA:O	1:B:238:GLU:HB3	2.14	0.47
1:A:314:MET:HE1	1:B:391:LEU:HD11	1.97	0.47
1:B:328:ASP:HA	1:B:329:PRO:HD2	1.75	0.47
1:A:235:LEU:HG	1:A:240:LEU:HD23	1.97	0.46
1:A:140:GLU:HG3	1:A:157:MET:HE1	1.97	0.46
1:A:84:LYS:HG3	1:A:85:VAL:N	2.31	0.46
1:B:280:ASN:OD1	1:B:341:PHE:HA	2.15	0.46
1:B:268:PHE:CD1	1:B:390:LEU:HD13	2.52	0.45
1:A:380:ILE:HD11	1:B:296:SER:H	1.81	0.45
1:A:69:LYS:HE2	1:A:73:ASP:OD2	2.16	0.45
1:B:53:HIS:O	1:B:56:ASP:HB2	2.16	0.45
1:B:180:GLU:HA	1:B:181:PRO:HD3	1.74	0.44
1:A:55:ASN:HA	1:A:58:ILE:O	2.18	0.44
1:A:158:ARG:HB3	3:A:471(A):HOH:O	2.16	0.44
1:A:217:THR:HA	1:A:227:PHE:CD1	2.53	0.44
1:B:303:GLY:HA2	1:B:306:ASP:HB2	1.99	0.44
1:B:387:ILE:O	1:B:391:LEU:HG	2.18	0.44
1:B:221:GLN:HE21	1:B:248:GLN:HB3	1.83	0.43
1:A:181:PRO:HA	3:A:484(A):HOH:O	2.18	0.43
1:B:35:PRO:O	1:B:39:VAL:HG23	2.19	0.43
1:B:208:GLY:HA3	3:B:602(B):HOH:O	2.19	0.43
1:B:195:VAL:HG13	1:B:213:LEU:HD11	2.01	0.43
1:A:37:GLU:O	1:A:41:LYS:HB2	2.19	0.42
1:B:131:GLU:HG3	3:B:711(B):HOH:O	2.17	0.42
1:A:182:LYS:HD2	1:A:219:HIS:CE1	2.54	0.42
1:B:108:ARG:O	1:B:112:ARG:HG3	2.19	0.42
1:B:61:ASP:O	1:B:62:ALA:C	2.62	0.42
1:A:180:GLU:HG3	1:A:214:ASN:O	2.20	0.42
1:A:53:HIS:O	1:A:54:ASP:C	2.62	0.42
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.85	0.42
1:A:380:ILE:HD11	1:B:296:SER:N	2.34	0.42
1:B:53:HIS:HA	1:B:89:THR:O	2.20	0.42
1:A:135:MET:HE2	1:A:177:ILE:HD13	2.02	0.41
1:B:184:ASN:C	1:B:184:ASN:ND2	2.79	0.41
1:B:377:PHE:O	1:B:378:ALA:HB3	2.21	0.41
1:A:40:HIS:HA	1:A:81:THR:HG21	2.02	0.41
1:A:87:MET:HA	1:A:132:THR:O	2.21	0.41
1:A:215:PRO:HG2	1:A:231:ILE:HG22	2.04	0.40
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LEU:CD2	3:B:445(B):HOH:O[4_555]	1.93	0.27
3:A:472(A):HOH:O	3:A:722(A):HOH:O[4_555]	2.05	0.15

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	391/394 (99%)	374 (96%)	16 (4%)	1 (0%)	36	55
1	B	391/394 (99%)	372 (95%)	16 (4%)	3 (1%)	16	31
All	All	782/788 (99%)	746 (95%)	32 (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	6	PRO
1	B	3	GLN

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	305/310 (98%)	288 (94%)	17 (6%)	19	39
1	B	305/310 (98%)	289 (95%)	16 (5%)	21	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	610/620 (98%)	577 (95%)	33 (5%)	20	41

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	41	LYS
1	A	44	GLU
1	A	68	GLU
1	A	69	LYS
1	A	84	LYS
1	A	96	PRO
1	A	149	ASP
1	A	150	LEU
1	A	174	ASN
1	A	184	ASN
1	A	206	GLU
1	A	213	LEU
1	A	284	LYS
1	A	286	THR
1	A	313	SER
1	A	359	ASN
1	B	6	PRO
1	B	20	THR
1	B	41	LYS
1	B	66	GLU
1	B	94	SER
1	B	131	GLU
1	B	149	ASP
1	B	158	ARG
1	B	184	ASN
1	B	213	LEU
1	B	235	LEU
1	B	273	LEU
1	B	286	THR
1	B	333	GLU
1	B	357	LEU
1	B	370	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	95	HIS
1	A	174	ASN
1	A	184	ASN
1	A	214	ASN
1	A	221	GLN
1	A	383	ASN
1	A	384	GLN
1	B	32	ASN
1	B	95	HIS
1	B	184	ASN
1	B	221	GLN
1	B	383	ASN
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, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.