



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:14 AM UTC

PDB ID : 1XLI / pdb_00001xli
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

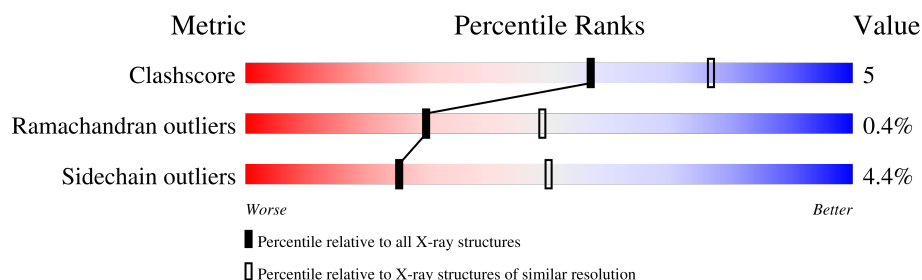
1 Overall quality at a glance

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](#)

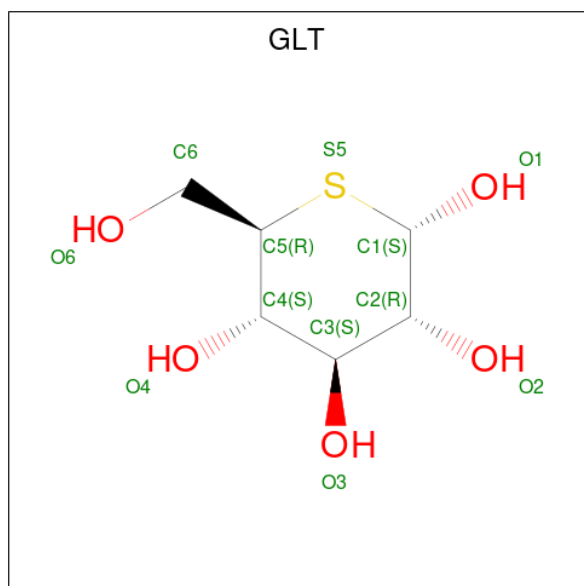
There are 4 unique types of molecules in this entry. The entry contains 6601 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 5-thio-alpha-D-glucopyranose (CCD ID: GLT) (formula: C₆H₁₂O₅S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			12	6	5	1		
2	B	1	Total	C	O	S	0	0
			12	6	5	1		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is water.

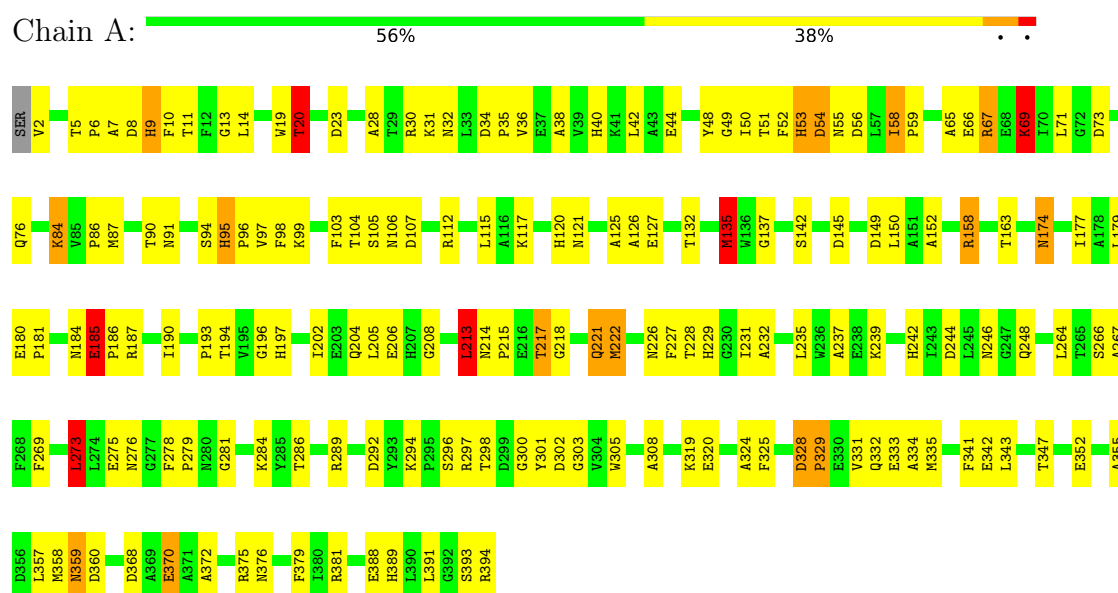
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	255	Total 255	O 255	0	0
4	B	264	Total 264	O 264	0	0

3 Residue-property plots

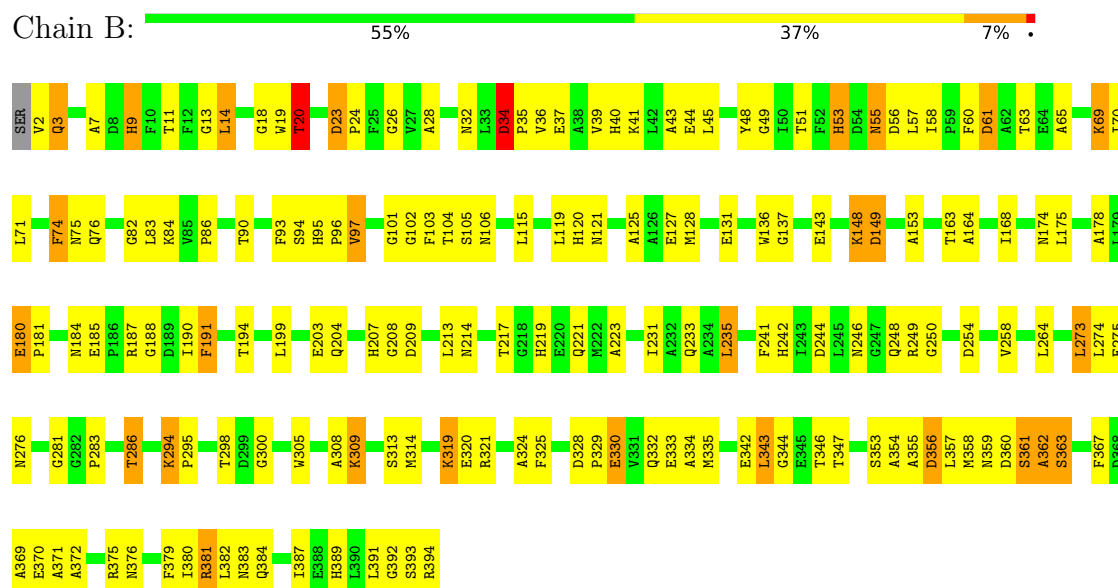
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	105.80 Å 105.80 Å 153.20 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}	0.150 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6601	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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, GLT

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	1.35	5/3101 (0.2%)	2.65	241/4204 (5.7%)
1	B	1.50	11/3101 (0.4%)	2.75	241/4204 (5.7%)
All	All	1.43	16/6202 (0.3%)	2.70	482/8408 (5.7%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	361	SER	C-N	32.56	1.75	1.33
1	B	362	ALA	N-CA	-7.15	1.37	1.46
1	B	101	GLY	C-N	-6.62	1.27	1.33
1	B	3	GLN	N-CA	-6.49	1.36	1.46
1	A	187	ARG	NE-CZ	5.95	1.39	1.33
1	B	233	GLN	C-O	5.75	1.30	1.24
1	B	300	GLY	N-CA	5.65	1.51	1.45
1	B	97	VAL	N-CA	-5.57	1.39	1.46
1	B	49	GLY	C-O	5.48	1.29	1.23
1	A	286	THR	CA-CB	5.43	1.61	1.53
1	B	23	ASP	N-CA	5.42	1.53	1.46
1	B	20	THR	C-O	5.35	1.31	1.24
1	A	394	ARG	CD-NE	-5.28	1.38	1.46
1	A	342	GLU	C-O	5.23	1.30	1.24
1	A	103	PHE	C-O	5.20	1.30	1.24
1	B	344	GLY	N-CA	-5.11	1.38	1.45

All (482) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	SER	CA-C-N	35.61	166.74	120.44
1	B	361	SER	C-N-CA	35.61	166.74	120.44
1	A	359	ASN	CA-CB-CG	30.24	142.84	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	CD-NE-CZ	25.18	159.66	124.40
1	B	356	ASP	O-C-N	-17.86	103.51	122.09
1	B	359	ASN	CA-CB-CG	15.28	127.88	112.60
1	B	2	VAL	CA-C-N	15.25	159.01	121.80
1	B	2	VAL	C-N-CA	15.25	159.01	121.80
1	B	362	ALA	N-CA-C	-15.15	94.85	111.07
1	A	6	PRO	CA-C-N	14.69	141.43	120.28
1	A	6	PRO	C-N-CA	14.69	141.43	120.28
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	356	ASP	CA-C-N	13.36	139.26	120.29
1	B	356	ASP	C-N-CA	13.36	139.26	120.29
1	A	244	ASP	CA-CB-CG	13.24	125.84	112.60
1	A	379	PHE	CA-CB-CG	12.00	125.80	113.80
1	B	361	SER	O-C-N	-11.73	107.00	122.59
1	B	32	ASN	CA-CB-CG	-11.71	100.89	112.60
1	B	60	PHE	CA-C-N	11.63	138.00	120.31
1	B	60	PHE	C-N-CA	11.63	138.00	120.31
1	A	112	ARG	CD-NE-CZ	11.37	140.31	124.40
1	B	217	THR	CA-C-N	11.12	132.32	119.98
1	B	217	THR	C-N-CA	11.12	132.32	119.98
1	A	329	PRO	CA-C-N	10.93	134.65	120.44
1	A	329	PRO	C-N-CA	10.93	134.65	120.44
1	A	137	GLY	CA-C-N	10.79	133.63	120.14
1	A	137	GLY	C-N-CA	10.79	133.63	120.14
1	B	127	GLU	CA-CB-CG	10.45	134.99	114.10
1	A	342	GLU	CA-CB-CG	10.29	134.69	114.10
1	A	308	ALA	CA-C-O	10.26	131.59	120.82
1	A	301	TYR	CA-C-O	-10.14	108.84	120.20
1	A	370	GLU	CA-C-O	-9.95	109.87	120.42
1	B	246	ASN	OD1-CG-ND2	-9.72	112.88	122.60
1	A	235	LEU	CA-C-N	9.65	133.22	120.28
1	A	235	LEU	C-N-CA	9.65	133.22	120.28
1	B	187	ARG	NE-CZ-NH2	-9.61	110.55	119.20
1	A	103	PHE	CA-CB-CG	9.60	123.39	113.80
1	B	286	THR	N-CA-CB	-9.59	95.38	111.20
1	A	187	ARG	NE-CZ-NH2	-9.54	110.61	119.20
1	B	102	GLY	N-CA-C	-9.42	101.64	110.21
1	A	342	GLU	N-CA-CB	9.39	124.69	110.22
1	A	94	SER	CA-C-O	-9.32	109.89	120.24
1	A	7	ALA	CA-C-N	9.23	134.34	120.31
1	A	7	ALA	C-N-CA	9.23	134.34	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	ASP	N-CA-C	-9.07	94.55	108.96
1	B	37	GLU	CB-CG-CD	9.04	127.97	112.60
1	B	360	ASP	CA-C-O	8.90	130.59	120.98
1	B	20	THR	N-CA-CB	-8.89	96.50	110.46
1	B	372	ALA	O-C-N	-8.89	112.70	122.12
1	B	164	ALA	CA-C-N	8.87	131.98	120.44
1	B	164	ALA	C-N-CA	8.87	131.98	120.44
1	B	208	GLY	O-C-N	-8.86	113.06	122.19
1	A	214	ASN	CB-CG-ND2	8.75	129.52	116.40
1	A	221	GLN	CA-C-N	8.74	135.31	120.72
1	A	221	GLN	C-N-CA	8.74	135.31	120.72
1	A	235	LEU	CA-C-O	8.64	129.89	120.82
1	B	319	LYS	CA-C-N	8.64	132.80	120.79
1	B	319	LYS	C-N-CA	8.64	132.80	120.79
1	B	188	GLY	O-C-N	-8.56	113.96	122.18
1	B	208	GLY	CA-C-N	8.54	132.58	120.28
1	B	208	GLY	C-N-CA	8.54	132.58	120.28
1	A	19	TRP	CA-C-O	8.52	130.50	120.70
1	B	34	ASP	CB-CA-C	8.39	121.60	109.26
1	B	76	GLN	CA-C-N	8.33	131.79	120.54
1	B	76	GLN	C-N-CA	8.33	131.79	120.54
1	B	190	ILE	CA-C-O	-8.33	110.91	121.48
1	B	94	SER	N-CA-C	8.29	121.51	111.40
1	B	362	ALA	CA-C-O	-8.24	112.17	120.82
1	B	309	LYS	CA-C-N	8.23	131.30	120.28
1	B	309	LYS	C-N-CA	8.23	131.30	120.28
1	A	105	SER	CA-C-N	8.22	131.97	120.29
1	A	105	SER	C-N-CA	8.22	131.97	120.29
1	B	391	LEU	CA-C-N	8.16	135.48	120.87
1	B	391	LEU	C-N-CA	8.16	135.48	120.87
1	A	65	ALA	N-CA-C	-8.15	102.09	110.97
1	A	332	GLN	OE1-CD-NE2	-8.02	114.58	122.60
1	B	392	GLY	CA-C-N	7.99	134.25	120.58
1	B	392	GLY	C-N-CA	7.99	134.25	120.58
1	B	343	LEU	CA-C-N	7.99	135.00	120.79
1	B	343	LEU	C-N-CA	7.99	135.00	120.79
1	A	389	HIS	CA-CB-CG	-7.98	105.82	113.80
1	B	131	GLU	CB-CG-CD	7.98	126.17	112.60
1	A	215	PRO	CA-C-O	-7.94	111.99	121.67
1	B	355	ALA	CA-C-O	-7.92	112.03	120.42
1	B	23	ASP	CB-CA-C	7.91	125.76	110.17
1	A	341	PHE	CA-C-O	-7.88	110.49	119.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	ASP	CA-C-N	7.84	128.81	120.03
1	A	302	ASP	C-N-CA	7.84	128.81	120.03
1	B	308	ALA	CA-C-N	7.83	130.62	120.44
1	B	308	ALA	C-N-CA	7.83	130.62	120.44
1	A	301	TYR	N-CA-C	7.82	121.76	111.75
1	B	20	THR	CB-CA-C	7.80	124.69	109.72
1	B	103	PHE	CA-CB-CG	7.76	121.56	113.80
1	B	115	LEU	CB-CA-C	7.75	124.03	110.85
1	A	217	THR	CA-C-N	7.72	128.55	119.98
1	A	217	THR	C-N-CA	7.72	128.55	119.98
1	B	75	ASN	CA-CB-CG	-7.69	104.91	112.60
1	A	58	ILE	CA-C-O	7.64	125.06	119.25
1	A	32	ASN	CA-CB-CG	-7.64	104.96	112.60
1	B	207	HIS	CA-C-N	7.62	129.73	120.13
1	B	207	HIS	C-N-CA	7.62	129.73	120.13
1	A	294	LYS	CG-CD-CE	7.60	128.79	111.30
1	B	384	GLN	OE1-CD-NE2	-7.59	115.01	122.60
1	B	48	TYR	N-CA-CB	-7.57	99.42	110.47
1	B	244	ASP	CA-CB-CG	7.57	120.17	112.60
1	B	143	GLU	CA-C-O	7.56	127.95	119.41
1	A	375	ARG	NE-CZ-NH2	-7.54	112.41	119.20
1	B	102	GLY	CA-C-N	7.53	131.13	120.28
1	B	102	GLY	C-N-CA	7.53	131.13	120.28
1	A	266	SER	CA-C-N	7.47	130.63	120.54
1	A	266	SER	C-N-CA	7.47	130.63	120.54
1	B	335	MET	CA-C-N	7.46	130.14	120.44
1	B	335	MET	C-N-CA	7.46	130.14	120.44
1	B	346	THR	CA-CB-OG1	-7.42	98.47	109.60
1	A	51	THR	CA-CB-CG2	7.39	123.06	110.50
1	A	20	THR	CA-CB-OG1	-7.37	98.55	109.60
1	A	125	ALA	CA-C-N	7.30	129.93	120.44
1	A	125	ALA	C-N-CA	7.30	129.93	120.44
1	A	328	ASP	CA-C-O	7.28	126.69	119.49
1	B	298	THR	O-C-N	-7.26	112.70	122.43
1	B	389	HIS	CA-CB-CG	-7.23	106.57	113.80
1	B	235	LEU	CA-C-O	7.21	129.00	121.07
1	B	53	HIS	CA-CB-CG	7.21	121.00	113.80
1	A	149	ASP	N-CA-C	-7.20	95.89	108.20
1	B	223	ALA	CA-C-N	7.18	133.72	120.87
1	B	223	ALA	C-N-CA	7.18	133.72	120.87
1	A	53	HIS	N-CA-CB	7.16	122.33	110.52
1	A	66	GLU	O-C-N	-7.14	114.66	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	GLU	CA-C-N	7.14	130.18	120.54
1	B	37	GLU	C-N-CA	7.14	130.18	120.54
1	B	69	LYS	N-CA-C	-7.12	103.21	110.97
1	B	43	ALA	CA-C-O	-7.10	113.02	120.55
1	A	298	THR	CA-C-N	7.05	132.52	122.09
1	A	298	THR	C-N-CA	7.05	132.52	122.09
1	B	231	ILE	CA-C-N	7.04	129.60	120.44
1	B	231	ILE	C-N-CA	7.04	129.60	120.44
1	B	246	ASN	CB-CG-ND2	7.02	126.94	116.40
1	A	9	HIS	CA-CB-CG	-7.01	106.79	113.80
1	B	250	GLY	CA-C-O	7.01	129.02	122.57
1	A	65	ALA	CA-C-O	-7.01	113.64	121.00
1	B	93	PHE	CA-C-O	-7.00	110.49	118.47
1	B	32	ASN	CA-C-O	-6.99	113.89	121.44
1	A	34	ASP	CA-CB-CG	6.96	119.56	112.60
1	B	168	ILE	CA-C-O	6.92	128.47	121.27
1	A	239	LYS	CA-CB-CG	6.89	127.88	114.10
1	B	363	SER	CB-CA-C	6.89	121.81	110.17
1	B	34	ASP	CA-C-N	6.89	126.36	118.85
1	B	34	ASP	C-N-CA	6.89	126.36	118.85
1	A	23	ASP	CB-CA-C	6.88	123.72	110.17
1	B	36	VAL	CA-C-N	6.88	129.49	120.28
1	B	36	VAL	C-N-CA	6.88	129.49	120.28
1	A	359	ASN	CA-C-O	-6.87	113.14	120.42
1	B	55	ASN	CA-C-N	6.86	130.74	120.31
1	B	55	ASN	C-N-CA	6.86	130.74	120.31
1	A	120	HIS	CA-CB-CG	-6.84	106.95	113.80
1	A	31	LYS	CA-C-O	-6.84	113.94	121.87
1	A	352	GLU	N-CA-C	-6.81	98.11	109.07
1	A	394	ARG	NE-CZ-NH1	6.80	128.31	121.50
1	A	54	ASP	CA-C-O	-6.80	113.30	120.92
1	B	294	LYS	CA-CB-CG	6.80	127.70	114.10
1	A	358	MET	CA-C-N	6.79	129.94	120.29
1	A	358	MET	C-N-CA	6.79	129.94	120.29
1	A	297	ARG	CA-C-N	6.79	130.63	120.31
1	A	297	ARG	C-N-CA	6.79	130.63	120.31
1	A	107	ASP	CA-CB-CG	6.79	119.39	112.60
1	B	120	HIS	CA-CB-CG	-6.78	107.02	113.80
1	B	97	VAL	CA-CB-CG1	6.78	121.92	110.40
1	B	367	PHE	CA-C-N	-6.74	112.80	122.77
1	B	367	PHE	C-N-CA	-6.74	112.80	122.77
1	B	314	MET	O-C-N	6.73	129.00	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	PHE	CA-CB-CG	6.72	120.52	113.80
1	A	308	ALA	CA-C-N	6.71	129.82	120.29
1	A	308	ALA	C-N-CA	6.71	129.82	120.29
1	B	76	GLN	OE1-CD-NE2	6.71	129.31	122.60
1	A	84	LYS	CA-C-N	6.71	134.54	122.13
1	A	84	LYS	C-N-CA	6.71	134.54	122.13
1	B	387	ILE	N-CA-CB	6.70	118.39	110.55
1	A	20	THR	N-CA-CB	-6.67	99.53	110.40
1	B	363	SER	N-CA-C	6.65	122.21	113.30
1	A	149	ASP	N-CA-CB	6.64	121.32	110.37
1	B	209	ASP	CA-C-O	-6.63	112.61	120.10
1	A	174	ASN	N-CA-CB	6.61	120.21	110.49
1	A	6	PRO	O-C-N	-6.61	113.72	122.64
1	A	94	SER	N-CA-C	6.60	119.81	111.69
1	A	59	PRO	CA-C-N	6.56	128.97	120.44
1	A	59	PRO	C-N-CA	6.56	128.97	120.44
1	A	84	LYS	O-C-N	-6.53	115.04	122.68
1	A	303	GLY	O-C-N	-6.53	115.83	122.17
1	B	19	TRP	N-CA-CB	6.53	119.83	109.51
1	A	214	ASN	OD1-CG-ND2	-6.52	116.08	122.60
1	A	38	ALA	CA-C-N	6.52	129.31	120.77
1	A	38	ALA	C-N-CA	6.52	129.31	120.77
1	A	35	PRO	CA-C-N	6.52	128.77	120.56
1	A	35	PRO	C-N-CA	6.52	128.77	120.56
1	B	264	LEU	N-CA-C	6.52	118.38	111.28
1	A	235	LEU	O-C-N	-6.51	115.36	122.07
1	A	229	HIS	CA-C-N	6.49	127.02	119.94
1	A	229	HIS	C-N-CA	6.49	127.02	119.94
1	A	273	LEU	CA-C-O	-6.49	114.00	120.82
1	A	71	LEU	CA-C-N	6.48	127.13	119.94
1	A	71	LEU	C-N-CA	6.48	127.13	119.94
1	B	53	HIS	N-CA-CB	6.45	120.92	110.41
1	A	196	GLY	CA-C-N	6.44	128.91	120.28
1	A	196	GLY	C-N-CA	6.44	128.91	120.28
1	A	221	GLN	O-C-N	-6.43	113.81	122.43
1	A	96	PRO	O-C-N	-6.42	113.93	122.22
1	A	208	GLY	O-C-N	-6.41	115.43	122.68
1	A	320	GLU	CA-C-N	6.40	128.86	120.28
1	A	320	GLU	C-N-CA	6.40	128.86	120.28
1	A	376	ASN	N-CA-CB	6.40	119.88	110.35
1	A	372	ALA	O-C-N	-6.36	114.78	122.22
1	A	190	ILE	CA-C-O	-6.35	113.34	121.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	LEU	CA-C-N	6.35	131.32	120.72
1	B	14	LEU	C-N-CA	6.35	131.32	120.72
1	B	131	GLU	CA-C-O	6.35	126.58	119.41
1	A	297	ARG	NE-CZ-NH2	-6.34	113.49	119.20
1	A	281	GLY	CA-C-O	-6.33	116.00	122.59
1	B	137	GLY	CA-C-N	6.33	128.05	120.14
1	B	137	GLY	C-N-CA	6.33	128.05	120.14
1	A	190	ILE	O-C-N	6.32	129.56	122.98
1	A	342	GLU	CB-CA-C	-6.31	98.95	110.63
1	A	106	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	A	206	GLU	N-CA-CB	6.30	119.48	110.16
1	B	332	GLN	CA-C-N	6.29	129.22	120.29
1	B	332	GLN	C-N-CA	6.29	129.22	120.29
1	B	274	LEU	O-C-N	6.28	128.87	122.09
1	A	13	GLY	N-CA-C	-6.28	103.58	112.37
1	B	84	LYS	N-CA-C	-6.27	100.65	110.36
1	A	231	ILE	CA-C-N	6.25	129.17	120.29
1	A	231	ILE	C-N-CA	6.25	129.17	120.29
1	B	241	PHE	CA-CB-CG	6.25	120.05	113.80
1	A	276	ASN	OD1-CG-ND2	-6.25	116.36	122.60
1	B	119	LEU	CA-C-N	6.24	128.65	120.28
1	B	119	LEU	C-N-CA	6.24	128.65	120.28
1	B	71	LEU	CA-C-N	6.24	126.91	119.98
1	B	71	LEU	C-N-CA	6.24	126.91	119.98
1	A	115	LEU	CB-CA-C	6.24	121.45	110.85
1	B	188	GLY	CA-C-N	6.23	132.34	122.74
1	B	188	GLY	C-N-CA	6.23	132.34	122.74
1	B	121	ASN	CA-C-N	6.16	129.17	120.42
1	B	121	ASN	C-N-CA	6.16	129.17	120.42
1	A	357	LEU	CA-C-O	-6.15	113.90	120.42
1	A	142	SER	CA-C-O	-6.13	114.88	121.38
1	A	117	LYS	CA-C-N	6.10	128.37	120.56
1	A	117	LYS	C-N-CA	6.10	128.37	120.56
1	B	329	PRO	CB-CA-C	6.09	121.00	112.11
1	A	51	THR	CA-CB-OG1	-6.07	100.50	109.60
1	B	281	GLY	CA-C-O	-6.05	117.39	122.29
1	A	228	THR	CA-C-N	6.05	128.39	120.28
1	A	228	THR	C-N-CA	6.05	128.39	120.28
1	A	297	ARG	O-C-N	-6.05	114.38	122.43
1	A	10	PHE	CB-CA-C	6.03	119.67	109.84
1	A	179	LEU	O-C-N	6.01	130.14	123.16
1	A	20	THR	OG1-CB-CG2	6.00	121.31	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ASP	N-CA-C	6.00	118.78	111.82
1	B	90	THR	CA-CB-OG1	-6.00	100.60	109.60
1	B	2	VAL	CA-C-O	6.00	131.00	120.80
1	B	379	PHE	CA-CB-CG	5.98	119.78	113.80
1	A	289	ARG	CD-NE-CZ	5.98	132.77	124.40
1	B	204	GLN	OE1-CD-NE2	-5.97	116.62	122.60
1	A	359	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	B	44	GLU	N-CA-CB	5.92	118.83	110.12
1	B	103	PHE	CA-C-O	-5.92	113.41	120.10
1	B	163	THR	CA-CB-OG1	-5.92	100.71	109.60
1	B	376	ASN	OD1-CG-ND2	-5.92	116.69	122.60
1	B	40	HIS	CA-CB-CG	-5.91	107.89	113.80
1	A	333	GLU	CA-CB-CG	5.90	125.91	114.10
1	A	185	GLU	O-C-N	-5.90	114.54	121.32
1	B	221	GLN	CA-C-N	5.88	130.54	120.72
1	B	221	GLN	C-N-CA	5.88	130.54	120.72
1	A	279	PRO	O-C-N	-5.87	115.48	122.24
1	A	355	ALA	CA-C-N	5.85	128.05	120.44
1	A	355	ALA	C-N-CA	5.85	128.05	120.44
1	B	74	PHE	CA-CB-CG	-5.84	107.96	113.80
1	A	237	ALA	CA-C-N	5.84	130.45	122.34
1	A	237	ALA	C-N-CA	5.84	130.45	122.34
1	B	51	THR	CA-CB-CG2	5.81	120.37	110.50
1	A	297	ARG	CD-NE-CZ	5.80	132.52	124.40
1	B	362	ALA	CA-C-N	-5.78	113.53	122.49
1	B	362	ALA	C-N-CA	-5.78	113.53	122.49
1	B	178	ALA	O-C-N	-5.78	116.57	123.27
1	B	13	GLY	N-CA-C	-5.78	104.28	112.37
1	A	242	HIS	O-C-N	-5.77	116.81	122.99
1	B	65	ALA	N-CA-C	-5.77	104.89	111.07
1	A	163	THR	CA-C-N	5.77	128.01	120.28
1	A	163	THR	C-N-CA	5.77	128.01	120.28
1	B	383	ASN	CA-C-N	5.77	128.01	120.28
1	B	383	ASN	C-N-CA	5.77	128.01	120.28
1	A	347	THR	CA-CB-OG1	-5.76	100.96	109.60
1	A	127	GLU	CA-CB-CG	5.75	125.61	114.10
1	B	359	ASN	CB-CA-C	5.75	122.00	109.99
1	B	82	GLY	CA-C-O	-5.75	112.62	119.06
1	A	67	ARG	CB-CG-CD	5.74	124.50	111.30
1	A	42	LEU	CA-C-N	5.74	127.90	120.44
1	A	42	LEU	C-N-CA	5.74	127.90	120.44
1	A	65	ALA	CB-CA-C	5.74	119.80	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	MET	CA-C-N	5.74	131.55	122.60
1	A	222	MET	C-N-CA	5.74	131.55	122.60
1	B	258	VAL	O-C-N	5.74	128.53	122.62
1	B	283	PRO	CB-CA-C	5.72	118.45	110.95
1	B	324	ALA	CA-C-N	5.72	128.26	120.54
1	B	324	ALA	C-N-CA	5.72	128.26	120.54
1	A	76	GLN	CA-C-N	5.72	128.26	120.54
1	A	76	GLN	C-N-CA	5.72	128.26	120.54
1	A	135	MET	N-CA-CB	5.72	119.57	110.65
1	B	347	THR	CA-CB-OG1	-5.71	101.03	109.60
1	A	104	THR	CA-CB-OG1	-5.71	101.03	109.60
1	B	328	ASP	CA-C-O	5.71	125.11	119.51
1	B	354	ALA	CA-C-O	-5.71	114.82	120.82
1	B	106	ASN	CA-CB-CG	5.71	118.31	112.60
1	A	359	ASN	CB-CG-ND2	5.70	124.95	116.40
1	B	32	ASN	OD1-CG-ND2	5.70	128.30	122.60
1	A	292	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	56	ASP	N-CA-C	-5.69	105.16	111.36
1	A	213	LEU	CD1-CG-CD2	-5.68	98.30	110.80
1	A	334	ALA	CA-C-N	5.68	127.89	120.28
1	A	334	ALA	C-N-CA	5.68	127.89	120.28
1	A	49	GLY	O-C-N	5.68	130.02	123.44
1	B	321	ARG	NE-CZ-NH2	-5.67	114.09	119.20
1	B	360	ASP	O-C-N	-5.65	115.00	122.57
1	B	63	THR	CA-C-O	-5.64	115.06	121.72
1	A	264	LEU	N-CA-C	5.64	117.23	111.14
1	A	187	ARG	NE-CZ-NH1	5.63	127.14	121.50
1	A	246	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	A	370	GLU	N-CA-CB	5.62	118.48	110.16
1	B	334	ALA	CA-C-N	5.62	127.81	120.28
1	B	334	ALA	C-N-CA	5.62	127.81	120.28
1	B	333	GLU	CA-C-N	5.61	127.73	120.44
1	B	333	GLU	C-N-CA	5.61	127.73	120.44
1	B	18	GLY	CA-C-O	-5.60	111.73	119.01
1	B	249	ARG	O-C-N	-5.60	116.12	122.84
1	B	249	ARG	CD-NE-CZ	5.59	132.23	124.40
1	B	382	LEU	CA-C-O	-5.59	114.63	120.55
1	A	121	ASN	CA-CB-CG	-5.59	107.01	112.60
1	B	44	GLU	CG-CD-OE1	-5.58	105.56	118.40
1	A	343	LEU	CA-C-N	5.58	130.34	120.74
1	A	343	LEU	C-N-CA	5.58	130.34	120.74
1	A	370	GLU	CG-CD-OE1	-5.57	105.58	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	LYS	N-CA-C	5.56	118.14	109.52
1	B	358	MET	CA-C-O	5.56	126.66	120.82
1	A	297	ARG	CA-C-O	5.56	126.11	119.10
1	A	67	ARG	CD-NE-CZ	5.55	132.17	124.40
1	A	194	THR	CA-CB-CG2	5.54	119.93	110.50
1	A	40	HIS	CA-CB-CG	-5.54	108.26	113.80
1	A	267	ALA	CA-C-N	5.54	128.50	120.79
1	A	267	ALA	C-N-CA	5.54	128.50	120.79
1	A	342	GLU	CA-C-O	-5.53	113.85	120.10
1	A	19	TRP	CA-C-N	5.53	130.82	121.14
1	A	19	TRP	C-N-CA	5.53	130.82	121.14
1	B	369	ALA	O-C-N	-5.53	116.26	122.12
1	A	320	GLU	CG-CD-OE2	5.52	131.10	118.40
1	A	56	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	242	HIS	N-CA-C	-5.51	100.55	108.60
1	B	26	GLY	N-CA-C	5.50	119.11	110.91
1	A	324	ALA	CA-C-N	5.49	127.90	120.65
1	A	324	ALA	C-N-CA	5.49	127.90	120.65
1	A	105	SER	O-C-N	-5.48	116.07	122.81
1	A	193	PRO	N-CA-C	5.48	120.71	113.86
1	B	248	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	A	305	TRP	CA-C-N	5.48	127.89	120.44
1	A	305	TRP	C-N-CA	5.48	127.89	120.44
1	B	190	ILE	O-C-N	5.47	128.93	122.69
1	A	120	HIS	O-C-N	-5.47	116.44	122.07
1	A	393	SER	N-CA-C	-5.46	106.62	113.72
1	A	5	THR	O-C-N	-5.46	117.29	121.55
1	B	69	LYS	CA-CB-CG	5.46	125.02	114.10
1	B	325	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	127	GLU	CB-CG-CD	-5.45	103.33	112.60
1	B	313	SER	CA-C-N	5.45	127.53	120.44
1	B	313	SER	C-N-CA	5.45	127.53	120.44
1	B	125	ALA	CA-C-N	5.44	127.51	120.44
1	B	125	ALA	C-N-CA	5.44	127.51	120.44
1	A	55	ASN	N-CA-C	5.44	119.66	113.19
1	B	20	THR	CA-CB-CG2	5.44	119.75	110.50
1	B	96	PRO	CA-C-N	5.44	129.06	120.47
1	B	96	PRO	C-N-CA	5.44	129.06	120.47
1	A	232	ALA	N-CA-C	-5.42	105.45	111.36
1	B	7	ALA	CA-C-N	5.42	129.77	120.72
1	B	7	ALA	C-N-CA	5.42	129.77	120.72
1	A	289	ARG	NE-CZ-NH2	-5.41	114.33	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	THR	CA-CB-CG2	5.41	119.70	110.50
1	A	269	PHE	CA-C-N	5.41	127.79	120.44
1	A	269	PHE	C-N-CA	5.41	127.79	120.44
1	A	36	VAL	CB-CA-C	5.40	118.88	111.97
1	B	381	ARG	CD-NE-CZ	-5.40	116.84	124.40
1	B	174	ASN	CA-C-N	5.39	131.64	122.37
1	B	174	ASN	C-N-CA	5.39	131.64	122.37
1	B	203	GLU	CA-C-N	5.38	131.42	122.54
1	B	203	GLU	C-N-CA	5.38	131.42	122.54
1	B	70	ILE	N-CA-C	5.38	116.01	110.36
1	A	388	GLU	CA-C-O	-5.38	114.85	120.55
1	B	320	GLU	CB-CG-CD	5.38	121.74	112.60
1	B	180	GLU	O-C-N	5.37	127.24	121.12
1	B	254	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	128	MET	CG-SD-CE	5.35	112.67	100.90
1	B	305	TRP	CB-CA-C	5.35	119.67	110.79
1	A	48	TYR	N-CA-C	-5.34	105.02	112.45
1	A	300	GLY	CA-C-O	-5.33	113.14	122.20
1	A	376	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	A	44	GLU	N-CA-CB	5.32	118.52	110.28
1	B	207	HIS	O-C-N	-5.31	115.40	122.20
1	B	180	GLU	CG-CD-OE1	5.31	130.61	118.40
1	B	199	LEU	CA-C-N	5.31	127.34	120.44
1	B	199	LEU	C-N-CA	5.31	127.34	120.44
1	B	298	THR	CA-C-N	5.31	131.67	122.64
1	B	298	THR	C-N-CA	5.31	131.67	122.64
1	B	121	ASN	CA-CB-CG	-5.30	107.30	112.60
1	B	330	GLU	CB-CG-CD	5.29	121.60	112.60
1	B	213	LEU	CA-CB-CG	5.28	134.79	116.30
1	B	342	GLU	CG-CD-OE2	-5.28	106.25	118.40
1	A	226	ASN	CA-C-N	5.26	127.65	120.54
1	A	226	ASN	C-N-CA	5.26	127.65	120.54
1	B	149	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	273	LEU	CA-CB-CG	5.26	134.71	116.30
1	A	98	PHE	CA-C-N	5.25	127.84	120.28
1	A	98	PHE	C-N-CA	5.25	127.84	120.28
1	A	145	ASP	CA-C-O	-5.25	112.92	119.38
1	B	309	LYS	CA-C-O	5.25	126.33	120.82
1	A	152	ALA	CA-C-O	-5.25	113.94	119.97
1	A	54	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	58	ILE	N-CA-C	5.24	112.74	107.55
1	B	235	LEU	O-C-N	-5.24	116.48	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	NE-CZ-NH2	-5.23	114.50	119.20
1	A	55	ASN	CA-C-N	5.23	127.71	120.29
1	A	55	ASN	C-N-CA	5.23	127.71	120.29
1	B	375	ARG	NE-CZ-NH2	-5.22	114.50	119.20
1	A	391	LEU	CA-C-N	5.21	131.61	121.41
1	A	391	LEU	C-N-CA	5.21	131.61	121.41
1	B	84	LYS	CA-C-N	5.21	131.76	122.13
1	B	84	LYS	C-N-CA	5.21	131.76	122.13
1	B	131	GLU	CG-CD-OE1	5.21	130.38	118.40
1	A	197	HIS	CA-C-N	5.19	125.71	119.94
1	A	197	HIS	C-N-CA	5.19	125.71	119.94
1	B	187	ARG	NH1-CZ-NH2	5.19	126.05	119.30
1	B	273	LEU	CA-CB-CG	5.19	134.46	116.30
1	B	101	GLY	CA-C-O	-5.18	117.13	122.26
1	A	126	ALA	CA-C-N	5.17	127.21	120.28
1	A	126	ALA	C-N-CA	5.17	127.21	120.28
1	A	206	GLU	N-CA-C	-5.17	105.72	111.36
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	A	292	ASP	O-C-N	5.17	128.12	122.64
1	B	354	ALA	N-CA-C	-5.16	105.55	111.07
1	B	175	LEU	CB-CA-C	-5.16	98.91	109.38
1	A	53	HIS	CA-CB-CG	5.16	118.96	113.80
1	A	30	ARG	CB-CG-CD	5.15	123.15	111.30
1	A	95	HIS	CA-C-N	5.14	124.94	119.28
1	A	95	HIS	C-N-CA	5.14	124.94	119.28
1	A	94	SER	O-C-N	5.12	128.89	122.23
1	B	219	HIS	CB-CG-CD2	5.12	137.85	131.20
1	B	219	HIS	CA-C-O	-5.12	115.43	120.70
1	B	371	ALA	CA-C-N	5.12	127.13	120.28
1	B	371	ALA	C-N-CA	5.12	127.13	120.28
1	B	153	ALA	CA-C-N	5.11	127.55	120.29
1	B	153	ALA	C-N-CA	5.11	127.55	120.29
1	A	52	PHE	O-C-N	5.11	128.62	123.26
1	A	23	ASP	CB-CG-OD1	5.11	130.14	118.40
1	A	91	ASN	CB-CG-ND2	-5.09	108.76	116.40
1	A	69	LYS	CA-C-O	5.09	126.35	121.00
1	B	9	HIS	CA-C-N	5.09	129.10	121.72
1	B	9	HIS	C-N-CA	5.09	129.10	121.72
1	A	67	ARG	NE-CZ-NH1	5.08	126.58	121.50
1	B	376	ASN	CB-CG-ND2	5.07	124.01	116.40
1	B	187	ARG	CB-CG-CD	5.07	122.96	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	ALA	N-CA-CB	5.06	117.35	110.01
1	A	328	ASP	CA-C-N	5.05	124.50	119.24
1	A	328	ASP	C-N-CA	5.05	124.50	119.24
1	B	90	THR	CA-C-O	-5.05	115.45	121.16
1	A	99	LYS	CA-C-O	-5.05	114.39	120.10
1	B	346	THR	CA-CB-CG2	5.04	119.07	110.50
1	B	393	SER	CA-C-O	-5.04	114.64	120.24
1	B	106	ASN	CA-C-N	5.04	128.50	121.24
1	B	106	ASN	C-N-CA	5.04	128.50	121.24
1	A	266	SER	CB-CA-C	5.04	118.79	110.88
1	B	231	ILE	CA-CB-CG1	5.03	118.95	110.40
1	B	207	HIS	CA-CB-CG	-5.02	108.78	113.80
1	A	368	ASP	CA-C-N	5.01	126.95	120.44
1	A	368	ASP	C-N-CA	5.01	126.95	120.44
1	A	360	ASP	CA-C-N	5.01	127.92	120.31
1	A	360	ASP	C-N-CA	5.01	127.92	120.31
1	B	191	PHE	CA-CB-CG	5.00	118.80	113.80

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	28	1
1	B	3027	0	2880	27	7
2	A	12	0	10	0	0
2	B	12	0	11	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	255	0	0	3	2
4	B	264	0	0	2	7
All	All	6601	0	5783	54	9

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 5.

All (54) 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:361:SER:C	1:B:362:ALA:N	1.75	1.43
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.58	0.82
1:A:58:ILE:HD13	1:A:67:ARG:HD2	1.73	0.71
1:A:95:HIS:HD2	1:A:97:VAL:H	1.41	0.67
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.76	0.67
1:B:95:HIS:HD2	1:B:97:VAL:H	1.41	0.66
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.78	0.66
1:A:158:ARG:HG3	1:A:205:LEU:HD23	1.82	0.62
1:B:45:LEU:HB3	1:B:309:LYS:HE3	1.83	0.59
1:A:84:LYS:HD2	4:A:424(A):HOH:O	2.03	0.58
1:A:69:LYS:HE2	1:A:73:ASP:OD2	2.05	0.57
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.88	0.56
1:B:20:THR:HG23	1:B:28:ALA:CB	2.36	0.56
1:B:23:ASP:HB2	1:B:24:PRO:HD2	1.88	0.55
1:B:55:ASN:HA	1:B:58:ILE:O	2.07	0.55
1:A:275:GLU:HG3	1:A:319:LYS:HG3	1.90	0.52
1:B:45:LEU:HD22	1:B:309:LYS:HE3	1.92	0.52
1:A:84:LYS:HB2	4:A:654(A):HOH:O	2.10	0.51
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.77	0.50
1:A:95:HIS:CD2	1:A:97:VAL:H	2.26	0.50
1:B:148:LYS:HG3	1:B:191:PHE:HZ	1.77	0.49
1:B:57:LEU:HD11	1:B:74:PHE:CD1	2.47	0.49
1:B:381:ARG:HD3	4:B:795(B):HOH:O	2.14	0.47
1:A:87:MET:HA	1:A:132:THR:O	2.15	0.47
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.96	0.47
1:B:20:THR:HG22	4:B:811(B):HOH:O	2.14	0.46
1:A:8:ASP:O	1:A:9:HIS:HB2	2.15	0.46
1:A:14:LEU:HD13	1:A:50:ILE:HD11	1.98	0.46
1:A:135:MET:HE2	1:A:177:ILE:HG21	1.98	0.45
1:A:296:SER:H	1:B:380:ILE:HD11	1.81	0.45
1:B:330:GLU:OE1	1:B:394:ARG:NH1	2.50	0.44
1:B:34:ASP:HA	1:B:35:PRO:HD3	1.79	0.44
1:B:14:LEU:HD21	1:B:35:PRO:HB3	2.00	0.44
1:B:180:GLU:HA	1:B:181:PRO:HD3	1.77	0.44
1:B:294:LYS:HA	1:B:295:PRO:HD3	1.86	0.43
1:B:23:ASP:CB	1:B:24:PRO:HD2	2.47	0.43
1:A:273:LEU:HD21	1:A:278:PHE:CE1	2.54	0.43
1:B:136:TRP:HB2	2:B:400:GLT:H61	1.99	0.43
1:B:53:HIS:O	1:B:56:ASP:HB2	2.19	0.43
1:A:217:THR:HA	1:A:227:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:GLY:O	1:A:222:MET:HG3	2.19	0.43
1:A:20:THR:HG23	1:A:28:ALA:CB	2.49	0.42
1:A:20:THR:HG23	1:A:28:ALA:HB2	1.99	0.42
1:A:158:ARG:HD3	1:A:204:GLN:O	2.19	0.42
1:A:331:VAL:O	1:A:335:MET:HG3	2.19	0.42
1:A:185:GLU:HA	1:A:186:PRO:HA	1.81	0.42
1:A:202:ILE:HD11	1:A:213:LEU:HD23	2.01	0.42
1:B:180:GLU:HG3	1:B:214:ASN:O	2.20	0.42
1:A:328:ASP:HA	1:A:329:PRO:HD3	1.86	0.42
1:A:180:GLU:HA	1:A:181:PRO:HD3	1.79	0.42
1:A:53:HIS:O	1:A:54:ASP:C	2.62	0.41
1:B:353:SER:H	1:B:356:ASP:HB2	1.83	0.41
1:A:381:ARG:HG3	4:A:593(A):HOH:O	2.21	0.41
1:B:35:PRO:O	1:B:39:VAL:HG23	2.20	0.40

All (9) 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:B:105:SER:CA	4:B:846(B):HOH:O[4_555]	1.16	1.04
1:B:105:SER:N	4:B:846(B):HOH:O[4_555]	1.32	0.88
4:A:564(A):HOH:O	4:B:668(B):HOH:O[4_555]	1.81	0.39
4:B:761(B):HOH:O	4:B:829(B):HOH:O[4_555]	1.90	0.30
1:B:104:THR:C	4:B:846(B):HOH:O[4_555]	1.92	0.28
1:A:69:LYS:NZ	1:B:276:ASN:O[6_665]	1.97	0.23
1:B:343:LEU:CD2	4:B:697(B):HOH:O[4_555]	2.05	0.15
1:B:9:HIS:CE1	4:A:648(A):HOH:O[6_655]	2.11	0.09
1:B:104:THR:O	4:B:846(B):HOH:O[4_555]	2.18	0.02

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%)	371 (95%)	19 (5%)	1 (0%)	36	55
1	B	391/394 (99%)	376 (96%)	13 (3%)	2 (0%)	24	43
All	All	782/788 (99%)	747 (96%)	32 (4%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU
1	B	3	GLN
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	305/310 (98%)	291 (95%)	14 (5%)	24	48
1	B	305/310 (98%)	292 (96%)	13 (4%)	26	51
All	All	610/620 (98%)	583 (96%)	27 (4%)	25	50

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

Mol	Chain	Res	Type
1	A	2	VAL
1	A	20	THR
1	A	69	LYS
1	A	90	THR
1	A	135	MET
1	A	150	LEU
1	A	158	ARG
1	A	174	ASN
1	A	184	ASN
1	A	213	LEU
1	A	273	LEU
1	A	284	LYS
1	A	359	ASN

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Mol	Chain	Res	Type
1	A	370	GLU
1	B	20	THR
1	B	34	ASP
1	B	41	LYS
1	B	61	ASP
1	B	69	LYS
1	B	149	ASP
1	B	184	ASN
1	B	235	LEU
1	B	273	LEU
1	B	286	THR
1	B	357	LEU
1	B	363	SER
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	9	HIS
1	A	75	ASN
1	A	95	HIS
1	A	120	HIS
1	A	174	ASN
1	A	221	GLN
1	A	383	ASN
1	A	384	GLN
1	B	40	HIS
1	B	76	GLN
1	B	95	HIS
1	B	120	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 ⓘ

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 6 ligands modelled in this entry, 4 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	GLT	B	400	3	11,12,12	1.04	1 (9%)	11,17,17	2.97	6 (54%)
2	GLT	A	400	3	11,12,12	1.81	3 (27%)	11,17,17	3.13	5 (45%)

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	GLT	B	400	3	-	0/2/22/22	0/1/1/1
2	GLT	A	400	3	-	2/2/22/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	GLT	C4-C5	-3.72	1.50	1.53
2	A	400	GLT	C5-S5	2.80	1.86	1.82
2	A	400	GLT	C6-C5	-2.04	1.50	1.52
2	B	400	GLT	C1-C2	-2.03	1.50	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	GLT	O3-C3-C2	6.38	125.42	110.38
2	B	400	GLT	C1-C2-C3	5.69	121.68	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	GLT	C1-C2-C3	5.30	120.91	110.55
2	A	400	GLT	C4-C3-C2	4.33	118.43	110.83
2	B	400	GLT	C4-C3-C2	3.78	117.47	110.83
2	B	400	GLT	O3-C3-C2	3.64	118.96	110.38
2	B	400	GLT	O4-C4-C5	-3.63	101.04	108.90
2	B	400	GLT	O1-C1-C2	2.99	116.67	110.03
2	A	400	GLT	O2-C2-C1	2.93	115.51	110.30
2	B	400	GLT	O2-C2-C1	2.64	114.99	110.30
2	A	400	GLT	O1-C1-C2	2.14	114.78	110.03

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	GLT	C4-C5-C6-O6
2	A	400	GLT	S5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	GLT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	361:SER	C	362:ALA	N	1.75

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.