



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:02 PM UTC

PDB ID : 1XLK / pdb_00001xllk
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

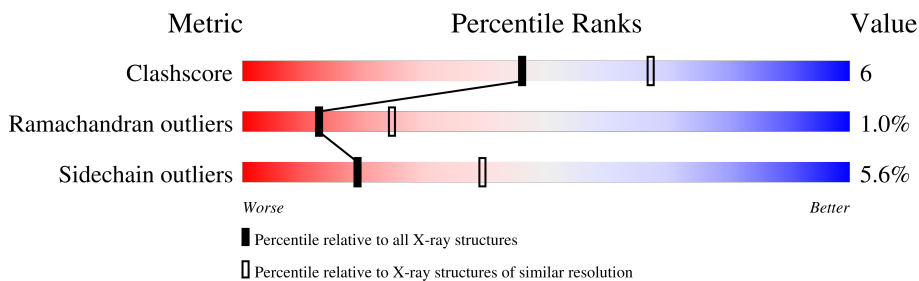
1 Overall quality at a glance

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	
1	B	394	

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.

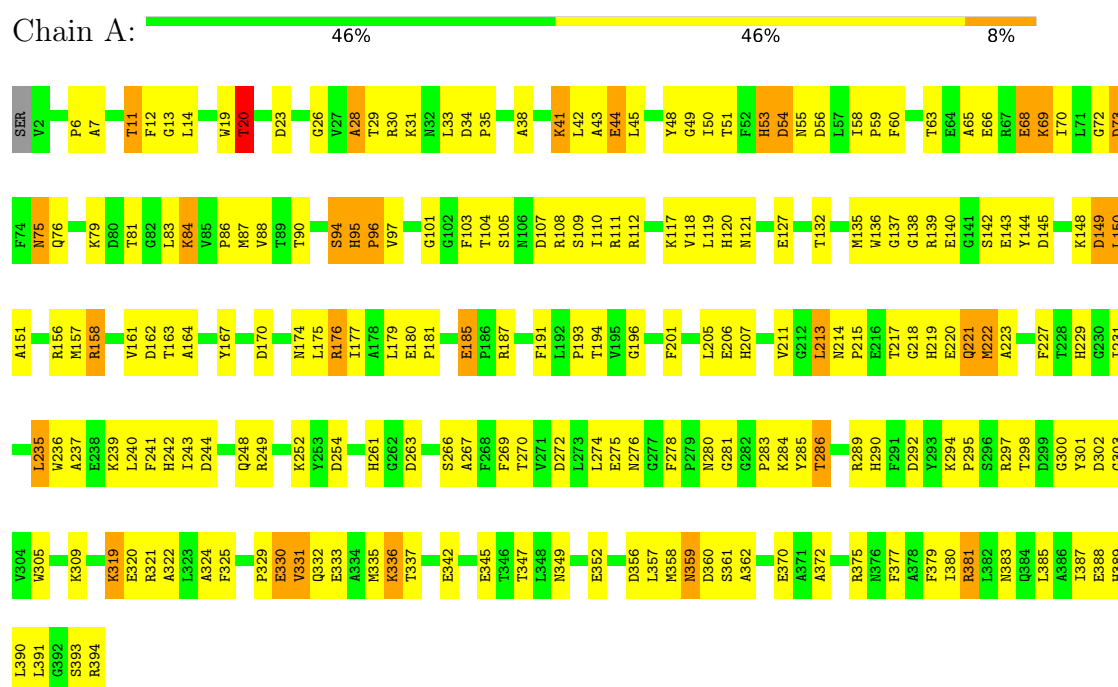
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	256	Total	O	0	0
			256	256		
3	B	266	Total	O	0	0
			266	266		

3 Residue-property plots

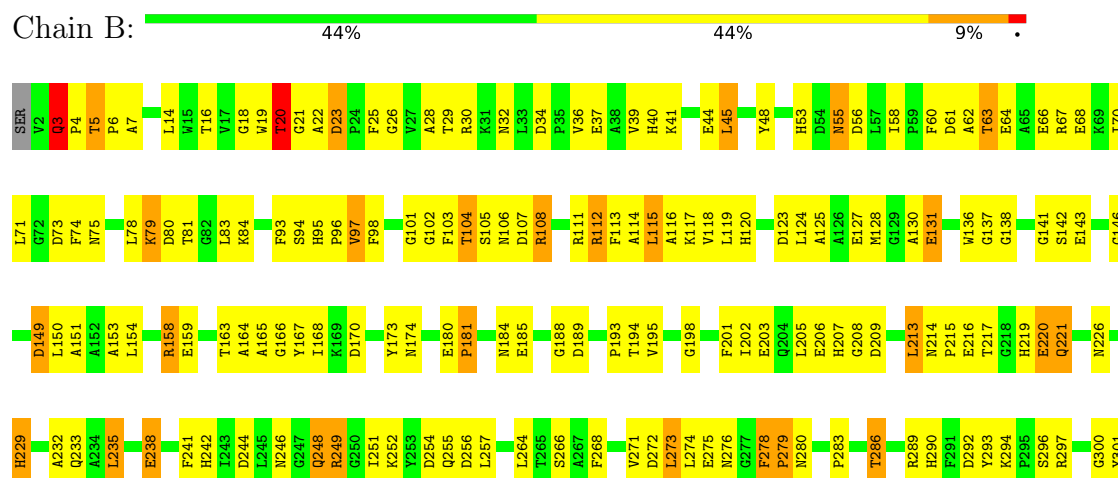
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

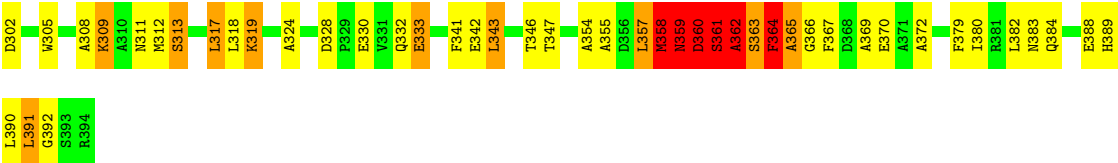
Note EDS was not executed.

• 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 154.30 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}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6580	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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

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	1.47	13/3101 (0.4%)	2.82	307/4204 (7.3%)
1	B	1.55	24/3101 (0.8%)	2.94	330/4204 (7.8%)
All	All	1.51	37/6202 (0.6%)	2.88	637/8408 (7.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	6

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	361	SER	CA-CB	-12.00	1.32	1.53
1	B	362	ALA	N-CA	-9.51	1.33	1.46
1	B	361	SER	C-N	-8.03	1.22	1.33
1	B	149	ASP	CA-CB	-6.60	1.44	1.53
1	B	193	PRO	C-O	6.53	1.32	1.24
1	A	158	ARG	CD-NE	-6.44	1.37	1.46
1	B	360	ASP	C-O	6.26	1.31	1.24
1	B	20	THR	N-CA	6.18	1.54	1.46
1	B	101	GLY	C-N	-6.18	1.28	1.33
1	A	103	PHE	C-O	5.93	1.31	1.24
1	B	359	ASN	N-CA	-5.89	1.38	1.46
1	B	300	GLY	N-CA	5.89	1.51	1.45
1	A	281	GLY	N-CA	5.86	1.51	1.45
1	B	81	THR	CA-CB	5.75	1.62	1.53
1	B	272	ASP	C-O	5.71	1.30	1.24
1	B	361	SER	N-CA	5.58	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	VAL	N-CA	-5.50	1.40	1.46
1	B	300	GLY	C-O	5.49	1.28	1.23
1	B	362	ALA	C-O	5.48	1.30	1.24
1	B	358	MET	C-N	-5.47	1.26	1.33
1	B	97	VAL	C-O	5.44	1.30	1.24
1	A	101	GLY	N-CA	5.43	1.51	1.45
1	B	102	GLY	CA-C	5.29	1.55	1.51
1	A	175	LEU	N-CA	-5.28	1.39	1.46
1	B	23	ASP	N-CA	5.27	1.53	1.46
1	B	202	ILE	C-O	5.27	1.30	1.24
1	B	14	LEU	C-O	5.22	1.30	1.24
1	A	394	ARG	NE-CZ	-5.22	1.27	1.33
1	B	251	ILE	CA-CB	5.21	1.59	1.53
1	A	227	PHE	C-O	5.14	1.30	1.24
1	B	233	GLN	C-O	5.12	1.30	1.24
1	A	300	GLY	N-CA	5.12	1.50	1.45
1	A	394	ARG	CD-NE	-5.12	1.39	1.46
1	A	94	SER	C-O	5.09	1.30	1.24
1	A	337	THR	CA-CB	5.04	1.61	1.53
1	A	13	GLY	N-CA	5.03	1.50	1.44
1	A	138	GLY	N-CA	-5.01	1.39	1.45

All (637) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	CD-NE-CZ	37.16	176.43	124.40
1	B	358	MET	CA-C-N	25.69	170.61	121.54
1	B	358	MET	C-N-CA	25.69	170.61	121.54
1	B	361	SER	N-CA-CB	24.68	151.10	110.87
1	B	361	SER	CA-C-N	20.89	161.45	121.54
1	B	361	SER	C-N-CA	20.89	161.45	121.54
1	A	112	ARG	CD-NE-CZ	18.64	150.50	124.40
1	B	359	ASN	CA-C-N	16.79	153.61	121.54
1	B	359	ASN	C-N-CA	16.79	153.61	121.54
1	A	158	ARG	CD-NE-CZ	16.74	147.84	124.40
1	A	6	PRO	CA-C-N	16.54	144.09	120.28
1	A	6	PRO	C-N-CA	16.54	144.09	120.28
1	B	357	LEU	O-C-N	-14.19	103.72	122.59
1	B	360	ASP	CA-C-O	-14.14	100.29	120.51
1	B	361	SER	CB-CA-C	-13.94	89.70	111.17
1	B	357	LEU	CA-C-N	13.41	147.16	121.54
1	B	357	LEU	C-N-CA	13.41	147.16	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ARG	NE-CZ-NH1	12.98	134.48	121.50
1	B	358	MET	N-CA-CB	12.83	132.17	110.49
1	A	73	ASP	CA-CB-CG	12.53	125.13	112.60
1	B	32	ASN	CA-CB-CG	-12.49	100.11	112.60
1	B	44	GLU	CA-CB-CG	12.46	139.03	114.10
1	A	379	PHE	CA-CB-CG	11.84	125.64	113.80
1	B	360	ASP	O-C-N	-11.33	107.53	122.59
1	A	145	ASP	CA-C-O	-11.32	106.95	119.97
1	B	137	GLY	CA-C-N	11.24	134.19	120.14
1	B	137	GLY	C-N-CA	11.24	134.19	120.14
1	A	56	ASP	CA-CB-CG	10.90	123.50	112.60
1	A	108	ARG	CD-NE-CZ	10.79	139.51	124.40
1	B	354	ALA	CA-C-O	-10.68	109.60	120.82
1	A	359	ASN	CA-CB-CG	10.63	123.23	112.60
1	A	137	GLY	CA-C-N	10.62	133.42	120.14
1	A	137	GLY	C-N-CA	10.62	133.42	120.14
1	B	392	GLY	CA-C-N	10.55	135.28	120.29
1	B	392	GLY	C-N-CA	10.55	135.28	120.29
1	B	20	THR	CB-CA-C	10.52	129.92	109.72
1	B	217	THR	CA-C-N	10.50	131.63	119.98
1	B	217	THR	C-N-CA	10.50	131.63	119.98
1	A	263	ASP	CA-CB-CG	10.45	123.05	112.60
1	A	289	ARG	CD-NE-CZ	10.35	138.89	124.40
1	A	112	ARG	NE-CZ-NH1	10.33	131.83	121.50
1	B	208	GLY	CA-C-N	10.30	134.49	120.38
1	B	208	GLY	C-N-CA	10.30	134.49	120.38
1	B	96	PRO	CA-C-N	10.18	134.41	120.46
1	B	96	PRO	C-N-CA	10.18	134.41	120.46
1	B	143	GLU	CA-C-O	10.17	130.90	119.41
1	B	20	THR	N-CA-CB	-10.07	94.65	110.46
1	B	60	PHE	CA-C-N	10.03	139.98	121.52
1	B	60	PHE	C-N-CA	10.03	139.98	121.52
1	A	222	MET	CA-C-N	9.98	137.96	122.49
1	A	222	MET	C-N-CA	9.98	137.96	122.49
1	A	283	PRO	CB-CA-C	9.97	123.98	111.12
1	B	208	GLY	O-C-N	-9.97	111.92	122.19
1	B	359	ASN	CB-CA-C	9.94	130.20	110.42
1	B	358	MET	CA-C-O	9.90	134.66	120.51
1	A	108	ARG	NE-CZ-NH2	-9.86	110.32	119.20
1	B	127	GLU	CA-CB-CG	9.72	133.55	114.10
1	B	93	PHE	CA-C-O	-9.64	107.48	118.47
1	A	103	PHE	CA-CB-CG	9.62	123.42	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	ASP	CA-C-N	-9.61	109.11	122.95
1	B	360	ASP	C-N-CA	-9.61	109.11	122.95
1	B	389	HIS	CA-CB-CG	-9.49	104.31	113.80
1	A	329	PRO	CA-C-N	9.46	132.73	120.44
1	A	329	PRO	C-N-CA	9.46	132.73	120.44
1	B	164	ALA	CA-C-N	9.43	132.70	120.44
1	B	164	ALA	C-N-CA	9.43	132.70	120.44
1	B	361	SER	CA-CB-OG	9.42	129.94	111.10
1	B	108	ARG	CD-NE-CZ	9.42	137.59	124.40
1	A	281	GLY	CA-C-O	-9.41	114.67	122.29
1	B	32	ASN	OD1-CG-ND2	9.37	131.97	122.60
1	B	20	THR	CA-CB-CG2	9.36	126.40	110.50
1	B	362	ALA	CA-C-O	-9.33	107.17	120.51
1	A	352	GLU	CA-C-O	-9.29	110.25	120.38
1	A	389	HIS	CA-CB-CG	-9.28	104.53	113.80
1	A	105	SER	CA-C-N	9.24	133.41	120.29
1	A	105	SER	C-N-CA	9.24	133.41	120.29
1	B	362	ALA	N-CA-C	-9.21	91.19	110.80
1	B	363	SER	N-CA-C	9.21	125.64	113.30
1	B	241	PHE	CA-CB-CG	8.94	122.74	113.80
1	B	391	LEU	CA-C-N	8.87	139.00	121.53
1	B	391	LEU	C-N-CA	8.87	139.00	121.53
1	B	359	ASN	CA-CB-CG	-8.85	103.75	112.60
1	B	165	ALA	CA-C-N	8.84	129.98	119.99
1	B	165	ALA	C-N-CA	8.84	129.98	119.99
1	A	94	SER	CA-C-O	-8.69	110.60	120.24
1	B	37	GLU	CB-CG-CD	8.68	127.35	112.60
1	B	297	ARG	NE-CZ-NH2	8.64	126.98	119.20
1	B	274	LEU	O-C-N	8.57	131.93	122.15
1	A	112	ARG	NE-CZ-NH2	-8.57	111.49	119.20
1	B	203	GLU	CA-C-N	8.57	136.68	122.54
1	B	203	GLU	C-N-CA	8.57	136.68	122.54
1	B	244	ASP	CA-CB-CG	8.54	121.14	112.60
1	A	342	GLU	CA-CB-CG	8.41	130.92	114.10
1	B	23	ASP	CB-CA-C	8.35	126.61	110.17
1	B	229	HIS	CA-C-N	8.33	129.19	119.94
1	B	229	HIS	C-N-CA	8.33	129.19	119.94
1	B	56	ASP	N-CA-CB	8.29	122.54	110.20
1	A	65	ALA	N-CA-C	-8.20	101.93	111.03
1	A	319	LYS	CA-C-N	8.16	131.04	120.44
1	A	319	LYS	C-N-CA	8.16	131.04	120.44
1	B	106	ASN	CA-C-N	8.14	132.96	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	ASN	C-N-CA	8.14	132.96	121.24
1	A	358	MET	CA-C-N	8.13	134.50	120.68
1	A	358	MET	C-N-CA	8.13	134.50	120.68
1	A	96	PRO	O-C-N	-8.11	112.36	122.17
1	B	346	THR	CA-CB-OG1	-8.11	97.43	109.60
1	A	231	ILE	CA-C-N	8.11	131.15	120.28
1	A	231	ILE	C-N-CA	8.11	131.15	120.28
1	B	114	ALA	CA-C-O	8.07	129.11	120.55
1	A	229	HIS	CA-C-N	8.06	128.73	119.94
1	A	229	HIS	C-N-CA	8.06	128.73	119.94
1	B	372	ALA	O-C-N	-7.92	113.72	122.12
1	B	149	ASP	CA-CB-CG	7.91	120.51	112.60
1	A	342	GLU	CB-CA-C	-7.89	96.03	110.63
1	B	286	THR	N-CA-CB	-7.87	98.22	111.20
1	A	164	ALA	CA-C-N	7.87	131.46	120.29
1	A	164	ALA	C-N-CA	7.87	131.46	120.29
1	B	384	GLN	OE1-CD-NE2	-7.86	114.74	122.60
1	A	51	THR	CA-CB-CG2	7.85	123.84	110.50
1	A	149	ASP	N-CA-C	-7.84	94.80	108.20
1	A	280	ASN	OD1-CG-ND2	-7.84	114.76	122.60
1	B	40	HIS	CA-CB-CG	-7.81	105.99	113.80
1	A	235	LEU	CA-C-O	7.80	129.01	120.82
1	B	36	VAL	CA-C-N	7.80	130.73	120.28
1	B	36	VAL	C-N-CA	7.80	130.73	120.28
1	A	6	PRO	O-C-N	-7.77	112.14	122.64
1	B	358	MET	CA-CB-CG	-7.77	98.56	114.10
1	B	248	GLN	OE1-CD-NE2	-7.72	114.88	122.60
1	B	354	ALA	N-CA-C	-7.69	102.84	111.07
1	A	117	LYS	CA-C-N	7.69	130.40	120.56
1	A	117	LYS	C-N-CA	7.69	130.40	120.56
1	A	20	THR	CB-CA-C	7.64	125.16	109.95
1	A	196	GLY	CA-C-N	7.60	130.47	120.28
1	A	196	GLY	C-N-CA	7.60	130.47	120.28
1	B	25	PHE	CA-CB-CG	-7.58	106.22	113.80
1	A	66	GLU	O-C-N	-7.56	114.22	122.09
1	B	103	PHE	CA-CB-CG	7.55	121.35	113.80
1	B	324	ALA	CA-C-N	7.55	130.71	120.44
1	B	324	ALA	C-N-CA	7.55	130.71	120.44
1	B	364	PHE	O-C-N	-7.53	112.57	122.59
1	B	318	LEU	CA-C-N	7.51	130.69	120.54
1	B	318	LEU	C-N-CA	7.51	130.69	120.54
1	A	330	GLU	CB-CA-C	-7.51	99.09	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	TRP	CA-C-O	-7.50	112.15	120.70
1	B	388	GLU	CA-C-N	7.47	130.90	120.29
1	B	388	GLU	C-N-CA	7.47	130.90	120.29
1	B	14	LEU	CA-C-O	7.44	128.44	120.55
1	B	214	ASN	CB-CG-ND2	7.43	127.55	116.40
1	B	242	HIS	CA-CB-CG	7.42	121.22	113.80
1	A	48	TYR	N-CA-C	-7.40	103.87	113.12
1	B	53	HIS	CA-CB-CG	7.39	121.19	113.80
1	B	363	SER	O-C-N	-7.36	113.33	122.24
1	B	141	GLY	CA-C-O	-7.36	115.22	121.04
1	A	156	ARG	CA-CB-CG	7.35	128.79	114.10
1	B	7	ALA	CA-C-N	7.34	131.47	120.31
1	B	7	ALA	C-N-CA	7.34	131.47	120.31
1	A	320	GLU	CA-CB-CG	7.32	128.73	114.10
1	A	292	ASP	CA-CB-CG	7.30	119.90	112.60
1	B	71	LEU	CA-C-N	7.29	127.89	119.94
1	B	71	LEU	C-N-CA	7.29	127.89	119.94
1	B	149	ASP	N-CA-C	-7.27	95.76	108.20
1	B	123	ASP	CA-C-O	-7.25	113.20	120.82
1	A	72	GLY	CA-C-N	7.19	129.78	120.44
1	A	72	GLY	C-N-CA	7.19	129.78	120.44
1	B	138	GLY	CA-C-O	-7.15	112.67	120.40
1	A	324	ALA	CA-C-N	7.12	130.05	120.65
1	A	324	ALA	C-N-CA	7.12	130.05	120.65
1	B	246	ASN	OD1-CG-ND2	-7.12	115.48	122.60
1	B	60	PHE	CA-CB-CG	7.08	120.88	113.80
1	B	254	ASP	CA-CB-CG	7.07	119.67	112.60
1	B	56	ASP	N-CA-C	-7.07	102.99	111.69
1	B	221	GLN	CA-C-N	7.07	132.53	120.72
1	B	221	GLN	C-N-CA	7.07	132.53	120.72
1	B	101	GLY	O-C-N	7.05	130.05	123.35
1	A	23	ASP	CA-CB-CG	7.05	119.65	112.60
1	B	114	ALA	N-CA-C	7.05	118.97	111.28
1	A	388	GLU	CA-C-O	-7.05	113.08	120.55
1	B	118	VAL	O-C-N	7.03	129.21	121.90
1	A	162	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	41	LYS	CA-C-N	7.00	130.23	120.29
1	A	41	LYS	C-N-CA	7.00	130.23	120.29
1	B	79	LYS	CA-C-O	7.00	128.77	121.07
1	B	383	ASN	CA-C-N	6.98	129.64	120.28
1	B	383	ASN	C-N-CA	6.98	129.64	120.28
1	A	143	GLU	CA-C-O	6.98	127.30	119.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	LEU	N-CA-C	-6.95	96.00	110.80
1	A	239	LYS	CA-CB-CG	6.94	127.98	114.10
1	A	352	GLU	N-CA-C	-6.91	97.94	109.07
1	A	149	ASP	N-CA-CB	6.90	121.75	110.37
1	A	201	PHE	CA-C-N	6.88	130.23	120.53
1	A	201	PHE	C-N-CA	6.88	130.23	120.53
1	A	59	PRO	CB-CA-C	6.88	120.03	111.23
1	B	142	SER	O-C-N	6.87	130.16	123.29
1	A	45	LEU	CA-C-O	-6.86	111.69	119.79
1	A	179	LEU	CA-C-O	-6.84	113.06	120.92
1	B	163	THR	CA-C-O	-6.83	113.67	120.70
1	B	300	GLY	O-C-N	-6.82	116.40	122.88
1	B	30	ARG	NE-CZ-NH2	-6.81	113.08	119.20
1	A	23	ASP	CB-CA-C	6.80	123.56	110.17
1	A	14	LEU	CA-C-O	6.78	127.61	120.42
1	A	175	LEU	O-C-N	6.78	131.54	123.27
1	B	3	GLN	CA-C-O	6.78	129.44	120.16
1	B	362	ALA	O-C-N	-6.77	113.59	122.59
1	A	336	LYS	CA-C-N	6.75	129.32	120.28
1	A	336	LYS	C-N-CA	6.75	129.32	120.28
1	A	301	TYR	N-CA-C	6.74	119.47	111.71
1	A	361	SER	N-CA-C	6.73	119.45	111.71
1	B	280	ASN	CA-C-O	-6.73	111.13	119.28
1	A	305	TRP	CA-C-N	6.72	129.18	120.44
1	A	305	TRP	C-N-CA	6.72	129.18	120.44
1	B	297	ARG	N-CA-CB	6.71	121.72	110.32
1	A	321	ARG	CA-C-N	6.70	129.93	120.28
1	A	321	ARG	C-N-CA	6.70	129.93	120.28
1	A	7	ALA	CA-C-N	6.67	132.03	120.68
1	A	7	ALA	C-N-CA	6.67	132.03	120.68
1	A	127	GLU	N-CA-CB	6.67	119.92	110.12
1	A	298	THR	CA-C-N	6.67	131.96	122.09
1	A	298	THR	C-N-CA	6.67	131.96	122.09
1	A	144	TYR	CA-C-O	6.66	127.89	120.70
1	A	394	ARG	CA-C-O	6.66	132.12	120.80
1	B	16	THR	CA-CB-OG1	-6.65	99.62	109.60
1	A	390	LEU	CA-C-N	6.65	134.55	121.58
1	A	390	LEU	C-N-CA	6.65	134.55	121.58
1	A	29	THR	CA-C-O	6.64	127.22	119.32
1	A	325	PHE	CA-CB-CG	6.63	120.43	113.80
1	B	302	ASP	N-CA-C	-6.63	104.13	111.36
1	B	313	SER	CA-C-N	6.62	129.48	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	SER	C-N-CA	6.62	129.48	120.54
1	B	289	ARG	NE-CZ-NH2	6.59	125.13	119.20
1	B	333	GLU	CA-C-N	6.58	129.00	120.44
1	B	333	GLU	C-N-CA	6.58	129.00	120.44
1	A	110	ILE	O-C-N	-6.57	115.47	121.91
1	A	20	THR	N-CA-CB	-6.55	99.40	110.41
1	B	380	ILE	N-CA-CB	6.55	118.96	110.57
1	B	56	ASP	CA-C-O	-6.55	112.97	120.24
1	B	308	ALA	CA-C-N	6.55	129.59	120.29
1	B	308	ALA	C-N-CA	6.55	129.59	120.29
1	A	167	TYR	O-C-N	-6.54	115.29	122.09
1	A	345	GLU	CB-CG-CD	6.54	123.72	112.60
1	B	16	THR	OG1-CB-CG2	6.54	122.38	109.30
1	A	95	HIS	CA-C-N	6.53	127.04	119.47
1	A	95	HIS	C-N-CA	6.53	127.04	119.47
1	A	295	PRO	CB-CA-C	6.52	118.66	111.56
1	A	179	LEU	O-C-N	6.50	130.71	123.16
1	A	381	ARG	CA-C-O	-6.50	113.67	120.55
1	B	379	PHE	CA-CB-CG	6.46	120.26	113.80
1	B	305	TRP	CA-C-N	6.46	128.83	120.44
1	B	305	TRP	C-N-CA	6.46	128.83	120.44
1	A	385	LEU	CA-C-O	-6.45	114.04	120.82
1	B	194	THR	CA-CB-CG2	6.45	121.46	110.50
1	A	381	ARG	NE-CZ-NH2	-6.44	113.41	119.20
1	A	244	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	142	SER	CA-C-O	-6.41	114.59	121.38
1	B	113	PHE	CA-C-O	-6.40	114.10	120.82
1	B	146	GLY	CA-C-N	6.39	131.39	120.72
1	B	146	GLY	C-N-CA	6.39	131.39	120.72
1	B	289	ARG	CB-CG-CD	6.39	125.99	111.30
1	A	196	GLY	O-C-N	-6.38	114.40	122.70
1	B	26	GLY	N-CA-C	6.38	121.15	110.56
1	B	219	HIS	CA-C-O	-6.38	114.13	120.70
1	B	276	ASN	CB-CG-ND2	6.37	125.96	116.40
1	B	68	GLU	CB-CA-C	6.37	122.90	110.67
1	A	237	ALA	CA-C-N	6.37	131.80	122.63
1	A	237	ALA	C-N-CA	6.37	131.80	122.63
1	A	54	ASP	CA-C-O	-6.37	113.57	121.02
1	A	297	ARG	CA-C-N	6.33	131.29	120.72
1	A	297	ARG	C-N-CA	6.33	131.29	120.72
1	B	108	ARG	NE-CZ-NH1	6.33	127.83	121.50
1	B	16	THR	CB-CA-C	6.32	121.28	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	GLU	N-CA-CB	6.30	120.05	110.28
1	A	266	SER	CA-C-N	6.30	128.62	120.44
1	A	266	SER	C-N-CA	6.30	128.62	120.44
1	A	342	GLU	N-CA-CB	6.25	119.85	110.22
1	B	384	GLN	CA-C-N	6.25	128.66	120.28
1	B	384	GLN	C-N-CA	6.25	128.66	120.28
1	B	364	PHE	CA-CB-CG	-6.25	107.55	113.80
1	A	372	ALA	CA-C-O	6.24	127.15	120.10
1	A	66	GLU	CA-C-N	6.24	128.64	120.28
1	A	66	GLU	C-N-CA	6.24	128.64	120.28
1	B	53	HIS	N-CA-CB	6.23	120.80	110.52
1	B	97	VAL	CA-CB-CG1	6.23	120.99	110.40
1	A	360	ASP	CA-C-N	6.22	129.24	120.28
1	A	360	ASP	C-N-CA	6.22	129.24	120.28
1	B	319	LYS	CA-C-N	6.22	128.53	120.44
1	B	319	LYS	C-N-CA	6.22	128.53	120.44
1	B	81	THR	CA-CB-OG1	-6.22	100.27	109.60
1	B	115	LEU	N-CA-C	-6.22	104.42	111.14
1	B	209	ASP	CA-CB-CG	6.21	118.81	112.60
1	B	45	LEU	CA-C-O	-6.21	111.74	119.38
1	A	26	GLY	O-C-N	6.21	129.54	123.76
1	B	112	ARG	CD-NE-CZ	6.20	133.08	124.40
1	B	150	LEU	CA-C-O	-6.19	113.11	120.10
1	B	383	ASN	CA-CB-CG	-6.16	106.44	112.60
1	A	267	ALA	CA-C-N	6.15	128.43	120.44
1	A	267	ALA	C-N-CA	6.15	128.43	120.44
1	A	59	PRO	CA-C-N	6.14	128.84	120.54
1	A	59	PRO	C-N-CA	6.14	128.84	120.54
1	A	139	ARG	NE-CZ-NH1	6.14	127.64	121.50
1	B	198	GLY	CA-C-N	6.13	128.50	120.28
1	B	198	GLY	C-N-CA	6.13	128.50	120.28
1	A	107	ASP	O-C-N	-6.12	115.25	122.96
1	A	111	ARG	CA-C-N	6.12	128.40	120.44
1	A	111	ARG	C-N-CA	6.12	128.40	120.44
1	A	120	HIS	O-C-N	-6.11	115.77	122.07
1	B	164	ALA	CA-C-O	-6.11	114.07	120.55
1	B	56	ASP	O-C-N	6.11	130.17	122.23
1	B	14	LEU	O-C-N	-6.09	115.66	122.12
1	A	28	ALA	CA-C-O	-6.08	114.87	121.44
1	A	322	ALA	CA-C-N	6.08	130.97	120.58
1	A	322	ALA	C-N-CA	6.08	130.97	120.58
1	A	241	PHE	CA-CB-CG	6.07	119.86	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ASP	CA-C-O	-6.07	115.28	122.13
1	A	65	ALA	CB-CA-C	6.06	120.35	110.95
1	B	232	ALA	CA-C-N	6.06	128.40	120.28
1	B	232	ALA	C-N-CA	6.06	128.40	120.28
1	A	84	LYS	O-C-N	-6.06	116.16	122.94
1	A	349	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	A	107	ASP	CA-C-O	6.05	127.59	120.58
1	A	84	LYS	N-CA-CB	-6.05	100.78	110.46
1	A	337	THR	CA-CB-OG1	-6.04	100.53	109.60
1	A	387	ILE	CA-C-N	6.04	128.38	120.28
1	A	387	ILE	C-N-CA	6.04	128.38	120.28
1	B	273	LEU	CA-CB-CG	6.04	137.43	116.30
1	A	34	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	107	ASP	CA-CB-CG	6.02	118.62	112.60
1	B	174	ASN	CB-CA-C	6.02	121.20	112.05
1	B	163	THR	CA-CB-OG1	-6.01	100.58	109.60
1	A	101	GLY	O-C-N	6.01	130.77	123.37
1	B	143	GLU	O-C-N	-6.01	113.83	122.36
1	A	207	HIS	O-C-N	-6.00	114.60	122.59
1	A	33	LEU	CA-C-O	-6.00	114.14	120.80
1	A	276	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	A	242	HIS	O-C-N	-5.99	116.98	123.26
1	B	34	ASP	CA-C-N	5.98	125.69	119.05
1	B	34	ASP	C-N-CA	5.98	125.69	119.05
1	A	278	PHE	CA-C-O	5.97	125.21	120.19
1	B	101	GLY	CA-C-O	-5.97	116.81	122.13
1	A	150	LEU	N-CA-C	5.96	118.74	111.82
1	A	337	THR	CB-CA-C	-5.96	100.90	110.79
1	B	22	ALA	O-C-N	5.95	130.00	123.04
1	A	19	TRP	CA-C-O	5.94	127.53	120.70
1	B	114	ALA	O-C-N	-5.93	115.83	122.12
1	B	96	PRO	O-C-N	-5.93	115.00	122.17
1	A	84	LYS	CB-CA-C	5.91	120.17	109.83
1	B	389	HIS	N-CA-CB	5.90	118.90	110.16
1	B	311	ASN	CA-C-N	5.90	128.46	120.44
1	B	311	ASN	C-N-CA	5.90	128.46	120.44
1	B	64	GLU	N-CA-CB	5.89	118.79	110.12
1	A	29	THR	CA-C-N	5.89	131.81	122.62
1	A	29	THR	C-N-CA	5.89	131.81	122.62
1	B	130	ALA	CA-C-O	-5.89	115.14	121.56
1	B	279	PRO	O-C-N	-5.89	114.69	122.64
1	A	286	THR	CA-C-O	-5.88	112.24	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	GLU	CA-C-N	5.87	128.07	120.44
1	B	64	GLU	C-N-CA	5.87	128.07	120.44
1	B	21	GLY	CA-C-N	-5.86	113.12	121.50
1	B	21	GLY	C-N-CA	-5.86	113.12	121.50
1	B	354	ALA	N-CA-CB	5.85	118.49	110.01
1	A	35	PRO	CA-C-N	5.84	127.92	120.56
1	A	35	PRO	C-N-CA	5.84	127.92	120.56
1	A	60	PHE	CA-C-N	5.84	132.95	122.38
1	A	60	PHE	C-N-CA	5.84	132.95	122.38
1	B	369	ALA	CA-C-O	5.84	126.61	120.42
1	A	285	TYR	CA-C-N	-5.84	113.18	122.29
1	A	285	TYR	C-N-CA	-5.84	113.18	122.29
1	A	309	LYS	CA-CB-CG	5.84	125.78	114.10
1	A	176	ARG	NH1-CZ-NH2	-5.83	111.72	119.30
1	A	149	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	272	ASP	CA-C-N	5.83	128.56	120.29
1	A	272	ASP	C-N-CA	5.83	128.56	120.29
1	B	238	GLU	CB-CG-CD	5.83	122.50	112.60
1	B	301	TYR	N-CA-C	5.83	119.49	112.38
1	A	88	VAL	CA-C-O	-5.82	114.53	121.28
1	A	121	ASN	CA-C-N	5.82	128.43	120.46
1	A	121	ASN	C-N-CA	5.82	128.43	120.46
1	B	207	HIS	CA-C-N	5.82	127.46	120.13
1	B	207	HIS	C-N-CA	5.82	127.46	120.13
1	A	278	PHE	CA-C-N	5.81	125.95	119.32
1	A	278	PHE	C-N-CA	5.81	125.95	119.32
1	B	369	ALA	O-C-N	-5.81	115.53	122.15
1	A	302	ASP	CA-C-N	5.81	126.42	119.98
1	A	302	ASP	C-N-CA	5.81	126.42	119.98
1	B	153	ALA	CA-C-O	-5.78	114.42	120.55
1	B	363	SER	N-CA-CB	-5.78	101.88	110.61
1	B	203	GLU	CG-CD-OE2	5.78	131.68	118.40
1	A	185	GLU	O-C-N	-5.77	114.68	121.32
1	A	206	GLU	N-CA-CB	5.77	118.38	110.01
1	B	170	ASP	CA-C-O	-5.77	114.40	120.63
1	B	32	ASN	CA-C-O	-5.76	115.22	121.44
1	B	102	GLY	N-CA-C	-5.76	104.96	110.21
1	B	206	GLU	CA-CB-CG	5.76	125.63	114.10
1	A	127	GLU	CB-CA-C	-5.76	101.23	110.79
1	B	271	VAL	CA-C-O	-5.76	114.96	120.95
1	A	94	SER	N-CA-C	5.74	118.74	111.69
1	B	53	HIS	N-CA-C	-5.74	100.36	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ARG	CG-CD-NE	5.73	124.61	112.00
1	A	121	ASN	O-C-N	-5.72	115.52	122.22
1	A	223	ALA	CA-C-N	5.72	130.73	120.77
1	A	223	ALA	C-N-CA	5.72	130.73	120.77
1	A	109	SER	N-CA-C	-5.72	104.96	111.14
1	A	75	ASN	CA-C-N	5.71	128.19	120.65
1	A	75	ASN	C-N-CA	5.71	128.19	120.65
1	B	125	ALA	CA-C-N	5.71	128.72	120.79
1	B	125	ALA	C-N-CA	5.71	128.72	120.79
1	B	107	ASP	CA-CB-CG	-5.70	106.90	112.60
1	B	220	GLU	O-C-N	-5.70	116.08	122.12
1	A	96	PRO	CA-C-N	5.70	128.26	120.46
1	A	96	PRO	C-N-CA	5.70	128.26	120.46
1	A	235	LEU	N-CA-CB	-5.69	101.76	110.01
1	B	181	PRO	CB-CA-C	5.68	118.76	110.63
1	B	317	LEU	CA-C-O	-5.68	114.39	120.42
1	A	109	SER	CB-CA-C	5.68	119.88	110.90
1	B	174	ASN	CA-C-N	5.67	132.13	122.37
1	B	174	ASN	C-N-CA	5.67	132.13	122.37
1	A	53	HIS	CB-CA-C	-5.67	99.96	109.48
1	B	48	TYR	N-CA-CB	-5.67	101.75	110.42
1	A	381	ARG	NE-CZ-NH1	5.66	127.16	121.50
1	A	105	SER	N-CA-C	-5.66	102.65	110.35
1	A	362	ALA	CA-C-N	5.66	130.30	120.68
1	A	362	ALA	C-N-CA	5.66	130.30	120.68
1	B	119	LEU	CA-C-N	5.66	127.86	120.28
1	B	119	LEU	C-N-CA	5.66	127.86	120.28
1	B	151	ALA	O-C-N	-5.66	115.70	122.15
1	B	367	PHE	CA-C-N	-5.66	114.99	122.85
1	B	367	PHE	C-N-CA	-5.66	114.99	122.85
1	A	236	TRP	CB-CA-C	5.64	120.15	110.79
1	A	333	GLU	CA-CB-CG	5.64	125.37	114.10
1	B	274	LEU	CA-C-O	-5.64	114.45	120.42
1	A	81	THR	CA-C-O	-5.63	112.68	119.27
1	B	19	TRP	CB-CA-C	-5.63	102.05	110.16
1	A	12	PHE	CA-C-O	-5.62	114.54	121.06
1	A	383	ASN	CA-CB-CG	-5.62	106.98	112.60
1	B	365	ALA	O-C-N	-5.62	116.29	122.07
1	B	113	PHE	N-CA-CB	5.61	118.15	110.01
1	A	53	HIS	N-CA-CB	5.61	119.78	110.52
1	B	93	PHE	O-C-N	5.59	128.51	121.64
1	B	369	ALA	CA-C-N	5.59	127.77	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	369	ALA	C-N-CA	5.59	127.77	120.28
1	B	44	GLU	CA-C-O	-5.57	113.57	119.97
1	A	270	THR	CA-CB-CG2	5.56	119.95	110.50
1	A	53	HIS	CA-C-O	-5.56	114.63	120.80
1	B	173	TYR	N-CA-CB	-5.56	102.17	110.17
1	A	56	ASP	CA-C-N	5.55	131.02	122.42
1	A	56	ASP	C-N-CA	5.55	131.02	122.42
1	B	342	GLU	CG-CD-OE2	-5.55	105.64	118.40
1	A	213	LEU	CD1-CG-CD2	-5.54	98.61	110.80
1	A	243	ILE	CA-C-O	-5.54	114.97	120.90
1	A	391	LEU	CA-C-N	5.53	132.25	121.41
1	A	391	LEU	C-N-CA	5.53	132.25	121.41
1	B	308	ALA	O-C-N	-5.53	116.26	122.12
1	A	26	GLY	N-CA-C	5.52	119.13	110.91
1	B	168	ILE	CA-C-N	5.51	127.98	120.54
1	B	168	ILE	C-N-CA	5.51	127.98	120.54
1	A	119	LEU	CA-C-N	5.51	127.60	120.44
1	A	119	LEU	C-N-CA	5.51	127.60	120.44
1	B	194	THR	CA-CB-OG1	-5.51	101.34	109.60
1	B	254	ASP	CB-CA-C	5.50	119.04	110.67
1	B	120	HIS	CA-C-N	5.50	128.67	120.31
1	B	120	HIS	C-N-CA	5.50	128.67	120.31
1	B	365	ALA	N-CA-C	5.49	116.95	111.07
1	A	194	THR	CA-C-N	5.49	127.68	120.60
1	A	194	THR	C-N-CA	5.49	127.68	120.60
1	B	5	THR	CA-C-N	5.49	126.70	119.84
1	B	5	THR	C-N-CA	5.49	126.70	119.84
1	B	278	PHE	N-CA-C	5.49	117.88	110.31
1	B	213	LEU	CA-CB-CG	5.48	135.49	116.30
1	B	355	ALA	CA-C-O	-5.48	115.07	120.82
1	B	361	SER	O-C-N	-5.48	114.66	122.99
1	B	305	TRP	CB-CA-C	5.47	121.18	110.67
1	A	75	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	B	84	LYS	N-CA-C	-5.46	102.67	110.59
1	A	139	ARG	NH1-CZ-NH2	-5.45	112.22	119.30
1	B	68	GLU	CB-CG-CD	5.43	121.84	112.60
1	A	194	THR	CA-CB-CG2	5.43	119.74	110.50
1	A	356	ASP	CA-C-N	5.42	127.82	120.44
1	A	356	ASP	C-N-CA	5.42	127.82	120.44
1	A	38	ALA	CA-C-N	5.42	127.60	120.60
1	A	38	ALA	C-N-CA	5.42	127.60	120.60
1	A	215	PRO	CA-C-O	-5.42	115.06	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	LYS	CG-CD-CE	5.41	123.75	111.30
1	A	95	HIS	CG-CD2-NE2	5.41	112.61	107.20
1	B	158	ARG	CB-CG-CD	5.41	123.74	111.30
1	B	249	ARG	CA-C-O	-5.41	116.02	122.13
1	A	193	PRO	N-CA-C	5.40	120.61	113.86
1	A	66	GLU	CB-CG-CD	5.40	121.78	112.60
1	A	170	ASP	CA-CB-CG	-5.40	107.20	112.60
1	B	312	MET	O-C-N	-5.39	116.26	122.09
1	A	109	SER	CA-C-O	-5.38	115.16	120.70
1	A	221	GLN	O-C-N	-5.38	115.03	122.46
1	A	393	SER	N-CA-C	-5.38	106.09	113.30
1	B	63	THR	CA-CB-OG1	-5.38	101.53	109.60
1	B	363	SER	CA-C-N	5.38	131.81	121.54
1	B	363	SER	C-N-CA	5.38	131.81	121.54
1	A	359	ASN	CA-C-O	-5.37	113.45	119.79
1	A	34	ASP	N-CA-C	-5.37	102.88	109.65
1	B	388	GLU	O-C-N	-5.37	116.43	122.12
1	A	276	ASN	CA-C-O	-5.37	112.24	119.11
1	B	106	ASN	N-CA-CB	5.37	118.60	110.28
1	A	20	THR	OG1-CB-CG2	5.36	120.03	109.30
1	B	167	TYR	CA-C-O	-5.36	115.19	120.82
1	B	286	THR	OG1-CB-CG2	5.36	120.03	109.30
1	B	127	GLU	O-C-N	-5.36	116.44	122.12
1	B	75	ASN	OD1-CG-ND2	5.36	127.96	122.60
1	B	98	PHE	CA-C-N	5.36	129.17	120.60
1	B	98	PHE	C-N-CA	5.36	129.17	120.60
1	B	143	GLU	CA-C-N	5.35	130.96	122.94
1	B	143	GLU	C-N-CA	5.35	130.96	122.94
1	A	163	THR	N-CA-CB	5.33	117.96	110.12
1	B	341	PHE	O-C-N	-5.33	115.30	122.23
1	A	68	GLU	CA-CB-CG	-5.33	103.44	114.10
1	B	18	GLY	CA-C-O	-5.33	112.08	119.01
1	B	61	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	274	LEU	O-C-N	5.33	128.22	122.15
1	A	118	VAL	CA-CB-CG1	5.32	119.44	110.40
1	A	333	GLU	CA-C-N	5.31	127.40	120.28
1	A	333	GLU	C-N-CA	5.31	127.40	120.28
1	B	328	ASP	O-C-N	5.31	126.12	121.18
1	A	104	THR	CA-CB-OG1	-5.30	101.65	109.60
1	A	269	PHE	CA-C-O	-5.30	112.86	119.38
1	B	312	MET	CA-C-N	5.30	128.16	120.79
1	B	312	MET	C-N-CA	5.30	128.16	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	HIS	CA-C-O	-5.30	115.77	121.38
1	B	359	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	B	173	TYR	CB-CA-C	5.29	119.28	109.54
1	B	347	THR	CA-CB-OG1	-5.29	101.67	109.60
1	A	375	ARG	NH1-CZ-NH2	5.28	126.16	119.30
1	B	332	GLN	CA-C-N	5.28	127.78	120.29
1	B	332	GLN	C-N-CA	5.28	127.78	120.29
1	B	346	THR	CA-CB-CG2	5.28	119.47	110.50
1	B	358	MET	O-C-N	-5.28	115.57	122.59
1	A	11	THR	CB-CA-C	5.27	119.72	109.33
1	A	249	ARG	NE-CZ-NH1	5.27	126.77	121.50
1	B	84	LYS	CA-C-N	5.27	131.88	122.13
1	B	84	LYS	C-N-CA	5.27	131.88	122.13
1	A	303	GLY	CA-C-N	5.26	127.19	120.56
1	A	303	GLY	C-N-CA	5.26	127.19	120.56
1	B	216	GLU	CB-CG-CD	5.26	121.53	112.60
1	A	63	THR	O-C-N	-5.25	116.24	122.65
1	B	257	LEU	CA-C-O	-5.25	115.94	121.88
1	B	372	ALA	CB-CA-C	5.25	119.51	110.79
1	B	382	LEU	CA-C-O	-5.25	114.98	120.55
1	A	290	HIS	CA-CB-CG	5.25	119.05	113.80
1	B	75	ASN	CA-C-O	-5.25	114.99	120.55
1	B	309	LYS	CA-CB-CG	5.25	124.59	114.10
1	B	19	TRP	N-CA-CB	5.24	117.80	109.51
1	B	297	ARG	CA-C-N	5.24	129.48	120.72
1	B	297	ARG	C-N-CA	5.24	129.48	120.72
1	B	117	LYS	CA-C-N	5.24	127.27	120.56
1	B	117	LYS	C-N-CA	5.24	127.27	120.56
1	B	64	GLU	CA-C-O	-5.23	115.00	120.55
1	B	136	TRP	CA-C-O	-5.23	114.87	120.46
1	B	343	LEU	CA-C-N	5.23	130.10	120.79
1	B	343	LEU	C-N-CA	5.23	130.10	120.79
1	A	136	TRP	N-CA-CB	5.23	119.29	110.46
1	A	76	GLN	CA-C-N	5.22	127.28	120.28
1	A	76	GLN	C-N-CA	5.22	127.28	120.28
1	A	44	GLU	CA-CB-CG	5.22	124.54	114.10
1	B	55	ASN	CA-C-N	5.22	129.50	120.58
1	B	55	ASN	C-N-CA	5.22	129.50	120.58
1	A	219	HIS	O-C-N	-5.21	116.70	122.07
1	B	215	PRO	CA-C-O	-5.21	115.52	121.56
1	B	294	LYS	CB-CA-C	-5.21	99.92	110.17
1	B	70	ILE	N-CA-CB	5.19	116.27	110.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	ARG	NH1-CZ-NH2	-5.19	112.55	119.30
1	A	70	ILE	CA-C-O	-5.18	115.88	121.27
1	B	290	HIS	CG-CD2-NE2	5.18	112.38	107.20
1	A	320	GLU	CG-CD-OE2	5.18	130.31	118.40
1	B	37	GLU	CA-C-N	5.18	127.48	120.44
1	B	37	GLU	C-N-CA	5.18	127.48	120.44
1	B	62	ALA	CA-C-O	5.18	126.66	121.07
1	B	255	GLN	CG-CD-NE2	5.18	124.17	116.40
1	B	206	GLU	N-CA-C	-5.17	105.55	111.14
1	A	269	PHE	CA-C-N	5.17	127.47	120.44
1	A	269	PHE	C-N-CA	5.17	127.47	120.44
1	A	331	VAL	CA-C-O	-5.17	115.38	120.85
1	B	32	ASN	N-CA-CB	-5.16	101.66	109.92
1	A	266	SER	CA-C-O	-5.16	115.09	120.55
1	A	332	GLN	CA-C-N	5.14	127.12	120.44
1	A	332	GLN	C-N-CA	5.14	127.12	120.44
1	A	31	LYS	CA-C-O	-5.14	115.91	121.87
1	A	23	ASP	CB-CG-OD1	5.13	130.20	118.40
1	A	176	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A	252	LYS	CA-C-N	5.13	128.36	120.82
1	A	252	LYS	C-N-CA	5.13	128.36	120.82
1	A	211	VAL	CA-CB-CG2	5.13	119.12	110.40
1	B	73	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	104	THR	OG1-CB-CG2	5.12	119.54	109.30
1	A	56	ASP	N-CA-CB	5.12	118.18	110.30
1	A	347	THR	CA-CB-CG2	5.11	119.19	110.50
1	B	264	LEU	N-CA-C	5.11	116.85	111.28
1	A	347	THR	CA-CB-OG1	-5.11	101.94	109.60
1	A	357	LEU	CA-C-O	-5.11	115.44	120.70
1	B	286	THR	CB-CA-C	5.11	119.29	111.02
1	A	254	ASP	CB-CA-C	5.10	119.04	110.88
1	A	79	LYS	N-CA-CB	5.10	117.40	110.01
1	B	189	ASP	CA-C-O	-5.10	114.66	120.32
1	A	370	GLU	CB-CG-CD	5.09	121.26	112.60
1	B	29	THR	CA-CB-OG1	-5.09	101.96	109.60
1	B	159	GLU	CA-CB-CG	5.09	124.28	114.10
1	B	330	GLU	CA-C-O	-5.09	114.12	119.97
1	A	221	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	A	151	ALA	N-CA-C	-5.08	105.44	111.69
1	A	261	HIS	CA-C-N	5.08	131.37	121.41
1	A	261	HIS	C-N-CA	5.08	131.37	121.41
1	A	161	VAL	O-C-N	-5.08	116.94	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	266	SER	CA-C-N	5.08	127.08	120.28
1	B	266	SER	C-N-CA	5.08	127.08	120.28
1	A	95	HIS	O-C-N	-5.08	115.95	121.53
1	A	303	GLY	O-C-N	-5.08	117.32	122.19
1	A	297	ARG	O-C-N	-5.07	115.68	122.43
1	A	223	ALA	CA-C-O	5.07	125.35	119.32
1	B	217	THR	CA-C-O	-5.07	115.09	121.02
1	B	297	ARG	CA-C-O	-5.07	113.36	119.49
1	A	42	LEU	CA-C-N	5.06	127.02	120.44
1	A	42	LEU	C-N-CA	5.06	127.02	120.44
1	B	255	GLN	O-C-N	-5.06	115.55	122.33
1	A	30	ARG	CD-NE-CZ	5.06	131.48	124.40
1	B	201	PHE	N-CA-CB	5.06	117.47	109.94
1	B	208	GLY	CA-C-O	5.06	125.61	120.45
1	A	23	ASP	CA-C-N	5.05	124.66	119.56
1	A	23	ASP	C-N-CA	5.05	124.66	119.56
1	A	217	THR	CA-C-N	5.05	126.64	120.22
1	A	217	THR	C-N-CA	5.05	126.64	120.22
1	B	166	GLY	N-CA-C	-5.05	106.53	112.64
1	B	188	GLY	CA-C-N	5.05	130.52	122.74
1	B	188	GLY	C-N-CA	5.05	130.52	122.74
1	A	220	GLU	CA-C-O	-5.04	115.07	120.42
1	A	297	ARG	CD-NE-CZ	5.04	131.46	124.40
1	A	375	ARG	CA-C-N	5.04	129.13	122.42
1	A	375	ARG	C-N-CA	5.04	129.13	122.42
1	B	154	LEU	CB-CA-C	5.04	119.41	110.85
1	A	187	ARG	NE-CZ-NH1	5.03	126.53	121.50
1	B	111	ARG	CA-C-N	5.03	127.02	120.28
1	B	111	ARG	C-N-CA	5.03	127.02	120.28
1	A	249	ARG	CD-NE-CZ	5.03	131.44	124.40
1	A	377	PHE	CA-C-O	-5.02	114.20	119.97
1	B	249	ARG	O-C-N	-5.01	116.89	122.55

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	358	MET	Peptide
1	B	359	ASN	Mainchain
1	B	361	SER	Mainchain,Peptide
1	B	362	ALA	Mainchain
1	B	364	PHE	Mainchain

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	32	0
1	B	3027	0	2880	38	12
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	256	0	0	6	0
3	B	266	0	0	3	5
All	All	6580	0	5762	69	12

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 (69) 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:HB3	1:B:366:GLY:H	1.40	0.85
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.70	0.72
1:A:95:HIS:HD2	1:A:97:VAL:H	1.37	0.72
1:B:357:LEU:HG	1:B:359:ASN:HA	1.75	0.67
1:B:95:HIS:HD2	1:B:97:VAL:H	1.44	0.64
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.81	0.63
1:A:135:MET:HE3	1:A:177:ILE:HG21	1.81	0.62
1:B:256:ASP:HB3	1:B:293:TYR:HA	1.81	0.62
1:A:275:GLU:HG3	1:A:319:LYS:HG3	1.82	0.61
1:B:361:SER:CB	1:B:364:PHE:H	2.14	0.60
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.68	0.57
1:A:84:LYS:HB2	3:A:660(A):HOH:O	2.03	0.57
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.86	0.57
1:B:131:GLU:HG3	3:B:649(B):HOH:O	2.04	0.56
1:A:380:ILE:HD11	1:B:296:SER:HB2	1.88	0.55
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.90	0.53
1:B:195:VAL:HG23	1:B:220:GLU:CD	2.34	0.53
1:A:95:HIS:CD2	1:A:97:VAL:H	2.24	0.53
1:B:361:SER:HB2	1:B:364:PHE:H	1.75	0.52
1:A:20:THR:HG23	1:A:28:ALA:CB	2.40	0.51
1:A:69:LYS:HE2	1:A:73:ASP:OD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:VAL:O	1:A:335:MET:HG3	2.11	0.50
1:B:361:SER:HB2	1:B:365:ALA:N	2.27	0.49
1:B:357:LEU:O	1:B:360:ASP:N	2.46	0.49
1:B:360:ASP:OD1	1:B:362:ALA:HB3	2.12	0.49
1:B:45:LEU:HB3	1:B:309:LYS:HE3	1.96	0.48
1:B:124:LEU:HD11	1:B:128:MET:HE2	1.95	0.47
1:B:361:SER:CB	1:B:366:GLY:H	2.18	0.47
1:A:336:LYS:HD3	3:A:635(A):HOH:O	2.14	0.47
1:B:45:LEU:HD22	1:B:309:LYS:HG2	1.96	0.47
1:B:20:THR:HG23	1:B:28:ALA:CB	2.45	0.47
1:B:79:LYS:O	1:B:80:ASP:C	2.55	0.47
1:B:55:ASN:HA	1:B:58:ILE:O	2.15	0.46
1:B:235:LEU:HD22	1:B:283:PRO:HB2	1.97	0.46
1:A:330:GLU:OE2	1:A:381:ARG:NH2	2.48	0.46
1:A:84:LYS:HD2	3:A:423(A):HOH:O	2.16	0.46
1:B:238:GLU:HG3	3:B:647(B):HOH:O	2.17	0.45
1:B:313:SER:O	1:B:317:LEU:HG	2.16	0.45
1:B:108:ARG:O	1:B:112:ARG:HG3	2.17	0.45
1:B:63:THR:HG23	1:B:66:GLU:OE2	2.17	0.45
1:A:53:HIS:O	1:A:54:ASP:C	2.61	0.44
1:A:218:GLY:O	1:A:222:MET:HG3	2.18	0.44
1:A:87:MET:HA	1:A:132:THR:O	2.18	0.44
1:A:180:GLU:HA	1:A:181:PRO:HD3	1.75	0.44
1:B:180:GLU:HA	1:B:181:PRO:HD3	1.78	0.43
1:A:11:THR:HA	1:A:49:GLY:O	2.19	0.43
1:A:20:THR:HG23	1:A:28:ALA:HB2	2.00	0.43
1:B:364:PHE:HB3	3:B:539(B):HOH:O	2.18	0.43
1:A:43:ALA:HB2	1:A:83:LEU:HD13	2.01	0.43
1:A:235:LEU:HG	1:A:240:LEU:HD23	1.99	0.43
1:A:55:ASN:HA	1:A:58:ILE:O	2.19	0.43
1:A:180:GLU:HG3	1:A:214:ASN:O	2.19	0.42
1:A:294:LYS:NZ	3:A:466(A):HOH:O	2.52	0.42
1:B:226:ASN:HB3	1:B:229:HIS:HB2	2.01	0.42
1:A:84:LYS:HG3	1:A:86:PRO:HG3	2.02	0.42
1:B:158:ARG:HG3	1:B:205:LEU:HD23	2.01	0.42
1:B:278:PHE:HA	1:B:279:PRO:HD3	1.88	0.42
1:B:249:ARG:O	1:B:252:LYS:HE3	2.21	0.41
1:A:20:THR:HG23	1:A:28:ALA:HB1	2.01	0.41
1:A:158:ARG:HB3	3:A:459(A):HOH:O	2.20	0.41
1:A:140:GLU:HG3	1:A:157:MET:HE1	2.02	0.41
1:A:158:ARG:HG2	1:A:205:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:PHE:CE2	1:B:78:LEU:HD11	2.56	0.41
1:B:268:PHE:CD1	1:B:390:LEU:HD13	2.55	0.41
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.86	0.40
1:A:75:ASN:ND2	3:A:561(A):HOH:O	2.53	0.40
1:B:221:GLN:HE21	1:B:248:GLN:HB3	1.85	0.40
1:B:3:GLN:HA	1:B:4:PRO:HD2	1.83	0.40
1:B:360:ASP:O	1:B:363:SER:N	2.51	0.40

All (12) 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:116:ALA:CA	1:B:359:ASN:OD1[4_555]	1.25	0.95
1:B:116:ALA:N	1:B:359:ASN:OD1[4_555]	1.30	0.90
1:B:116:ALA:CB	1:B:359:ASN:CB[4_555]	1.39	0.81
1:B:105:SER:CA	3:B:592(B):HOH:O[4_555]	1.53	0.67
1:B:105:SER:N	3:B:592(B):HOH:O[4_555]	1.63	0.57
1:B:116:ALA:CA	1:B:359:ASN:CG[4_555]	1.75	0.45
1:B:104:THR:C	3:B:592(B):HOH:O[4_555]	1.85	0.35
1:B:115:LEU:C	1:B:359:ASN:OD1[4_555]	1.92	0.28
1:B:343:LEU:CD2	3:B:438(B):HOH:O[4_555]	1.93	0.27
1:B:104:THR:O	3:B:592(B):HOH:O[4_555]	1.97	0.23
1:B:116:ALA:CA	1:B:359:ASN:CB[4_555]	2.05	0.15
1:B:116:ALA:CB	1:B:359:ASN:CG[4_555]	2.14	0.06

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%)	376 (96%)	14 (4%)	1 (0%)	36 55
1	B	391/394 (99%)	366 (94%)	18 (5%)	7 (2%)	6 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	782/788 (99%)	742 (95%)	32 (4%)	8 (1%)	12	24

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	358	MET
1	B	359	ASN
1	B	360	ASP
1	B	362	ALA
1	A	185	GLU
1	B	185	GLU
1	B	23	ASP
1	B	3	GLN

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%)	288 (94%)	17 (6%)	19	39
1	B	305/310 (98%)	288 (94%)	17 (6%)	19	39
All	All	610/620 (98%)	576 (94%)	34 (6%)	19	39

All (34) 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	50	ILE
1	A	68	GLU
1	A	69	LYS
1	A	90	THR
1	A	94	SER
1	A	96	PRO
1	A	149	ASP

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Mol	Chain	Res	Type
1	A	150	LEU
1	A	174	ASN
1	A	176	ARG
1	A	213	LEU
1	A	284	LYS
1	A	286	THR
1	A	359	ASN
1	B	5	THR
1	B	6	PRO
1	B	20	THR
1	B	41	LYS
1	B	94	SER
1	B	131	GLU
1	B	149	ASP
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	358	MET
1	B	360	ASP
1	B	370	GLU
1	B	391	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	53	HIS
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	359	ASN
1	A	383	ASN
1	A	384	GLN
1	B	95	HIS
1	B	221	GLN
1	B	359	ASN

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Mol	Chain	Res	Type
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.