



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:20 PM UTC

PDB ID : 1DID / pdb_00001did
Title : OBSERVATIONS OF REACTION INTERMEDIATES AND THE MECHANISM OF ALDOSE-KETOSE INTERCONVERSION BY D-XYLOSE ISOMERASE
Authors : Collyer, C.A.; Goldberg, J.D.; Blow, D.M.
Deposited on : 1992-06-04
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

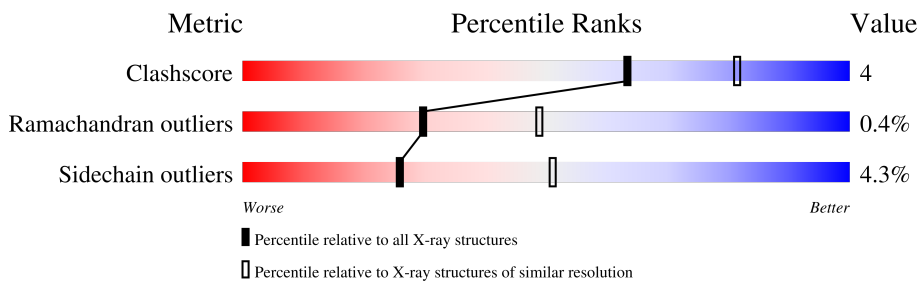
1 Overall quality at a glance

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](#)

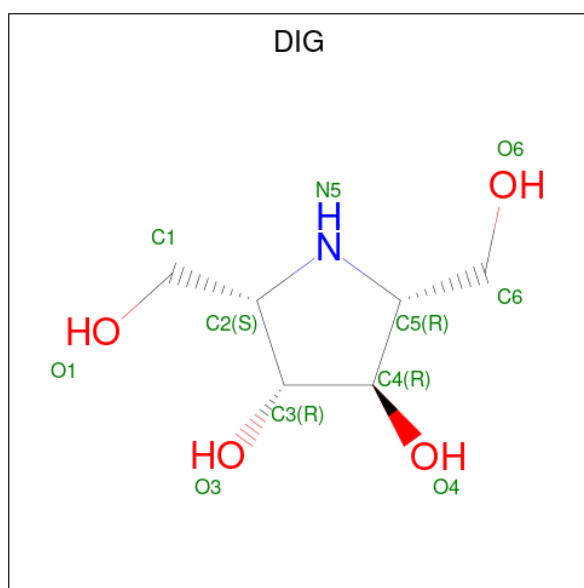
There are 4 unique types of molecules in this entry. The entry contains 6584 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2,5-DIDEOXY-2,5-IMINO-D-GLUCITOL (CCD ID: DIG) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	1	4		
2	B	1	Total	C	N	O	0	0
			11	6	1	4		

- 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.

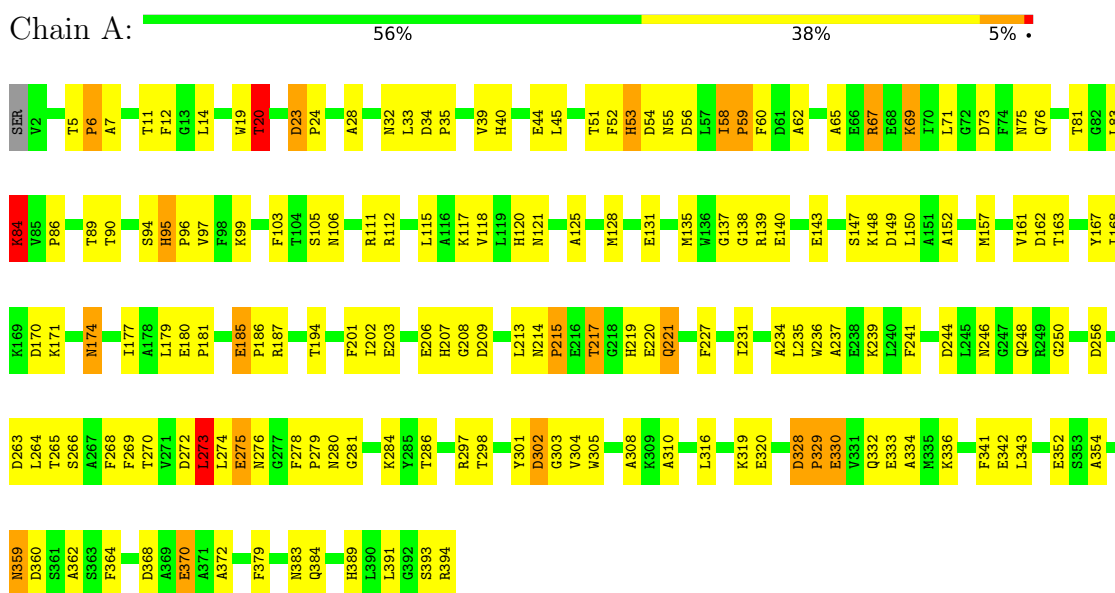
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	256	Total 256	O 256	0	0
4	B	248	Total 248	O 248	0	0

3 Residue-property plots

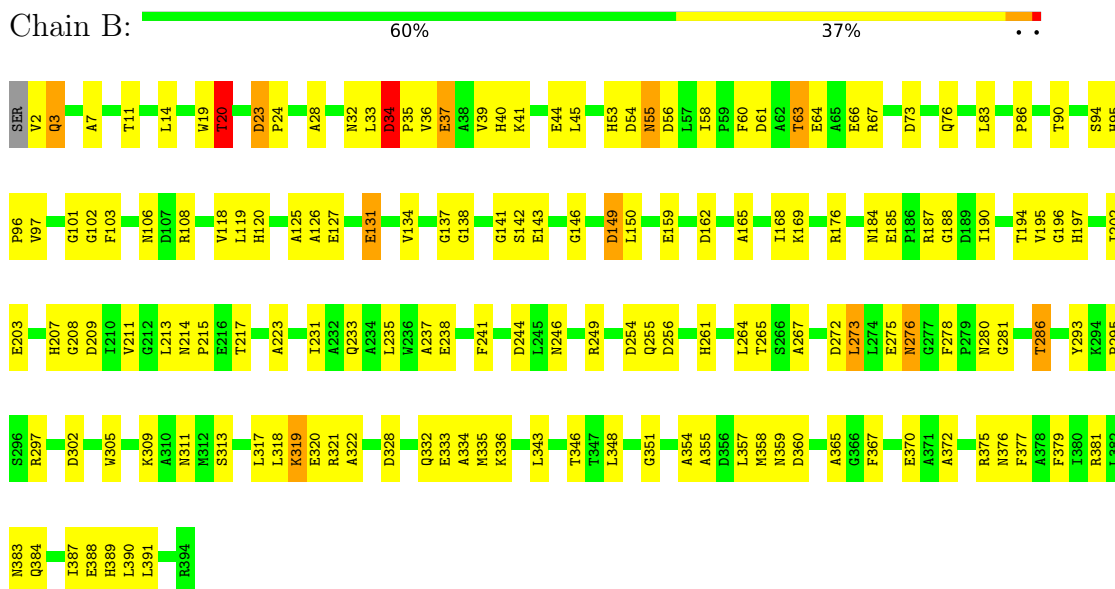
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	106.10Å 106.10Å 153.30Å 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}	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6584	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: DIG, 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	1.30	4/3101 (0.1%)	2.64	255/4204 (6.1%)
1	B	1.30	4/3101 (0.1%)	2.49	223/4204 (5.3%)
All	All	1.30	8/6202 (0.1%)	2.56	478/8408 (5.7%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	GLY	CA-C	8.30	1.57	1.51
1	B	101	GLY	C-N	-7.77	1.26	1.33
1	A	275	GLU	C-O	6.42	1.31	1.24
1	A	148	LYS	N-CA	-5.30	1.39	1.45
1	B	138	GLY	N-CA	-5.23	1.38	1.45
1	B	19	TRP	C-N	-5.15	1.26	1.33
1	A	286	THR	CA-CB	5.10	1.61	1.53
1	A	394	ARG	CD-NE	-5.03	1.39	1.46

All (478) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	CD-NE-CZ	21.51	154.51	124.40
1	A	6	PRO	CA-C-N	15.11	142.04	120.28
1	A	6	PRO	C-N-CA	15.11	142.04	120.28
1	B	73	ASP	CA-CB-CG	14.28	126.88	112.60
1	A	137	GLY	CA-C-N	13.71	135.39	120.03
1	A	137	GLY	C-N-CA	13.71	135.39	120.03
1	A	237	ALA	CA-C-N	11.64	138.53	122.34
1	A	237	ALA	C-N-CA	11.64	138.53	122.34
1	A	302	ASP	CA-C-N	11.11	132.31	119.98
1	A	302	ASP	C-N-CA	11.11	132.31	119.98
1	A	329	PRO	CA-C-N	10.97	134.70	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	PRO	C-N-CA	10.97	134.70	120.44
1	B	102	GLY	N-CA-C	-10.86	100.33	110.21
1	B	217	THR	CA-C-N	10.86	132.19	120.03
1	B	217	THR	C-N-CA	10.86	132.19	120.03
1	A	342	GLU	N-CA-CB	10.73	126.74	110.22
1	B	120	HIS	CA-CB-CG	-10.59	103.21	113.80
1	A	7	ALA	CA-C-N	10.55	136.34	120.31
1	A	7	ALA	C-N-CA	10.55	136.34	120.31
1	A	103	PHE	CA-CB-CG	10.39	124.19	113.80
1	B	381	ARG	NE-CZ-NH2	-10.30	109.93	119.20
1	A	394	ARG	NE-CZ-NH1	9.87	131.37	121.50
1	A	273	LEU	CA-C-O	-9.74	110.59	120.82
1	B	372	ALA	O-C-N	-9.66	111.88	122.12
1	B	246	ASN	OD1-CG-ND2	-9.56	113.04	122.60
1	A	308	ALA	CA-C-N	9.50	133.78	120.29
1	A	308	ALA	C-N-CA	9.50	133.78	120.29
1	A	328	ASP	CA-C-O	9.43	128.82	119.49
1	B	237	ALA	CA-C-N	9.39	135.39	122.34
1	B	237	ALA	C-N-CA	9.39	135.39	122.34
1	A	379	PHE	CA-CB-CG	9.15	122.95	113.80
1	B	286	THR	N-CA-CB	-9.04	96.06	110.98
1	B	32	ASN	CA-CB-CG	-9.03	103.57	112.60
1	A	105	SER	CA-C-N	8.99	133.06	120.29
1	A	105	SER	C-N-CA	8.99	133.06	120.29
1	B	56	ASP	CA-CB-CG	8.72	121.32	112.60
1	B	187	ARG	NE-CZ-NH2	-8.67	111.40	119.20
1	A	23	ASP	CA-CB-CG	8.65	121.25	112.60
1	A	297	ARG	CA-C-N	8.62	133.41	120.31
1	A	297	ARG	C-N-CA	8.62	133.41	120.31
1	A	342	GLU	CA-CB-CG	8.61	131.33	114.10
1	A	217	THR	CA-C-N	8.60	129.53	119.98
1	A	217	THR	C-N-CA	8.60	129.53	119.98
1	B	389	HIS	CA-CB-CG	-8.58	105.22	113.80
1	A	94	SER	N-CA-C	8.54	120.36	111.14
1	A	276	ASN	OD1-CG-ND2	-8.50	114.10	122.60
1	B	379	PHE	CA-CB-CG	8.28	122.08	113.80
1	B	384	GLN	OE1-CD-NE2	-8.25	114.35	122.60
1	A	163	THR	CA-C-N	8.19	131.26	120.28
1	A	163	THR	C-N-CA	8.19	131.26	120.28
1	A	148	LYS	CA-C-N	8.16	133.45	122.84
1	A	148	LYS	C-N-CA	8.16	133.45	122.84
1	A	106	ASN	OD1-CG-ND2	-8.13	114.47	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	ASP	CA-CB-CG	8.13	120.73	112.60
1	B	238	GLU	CA-CB-CG	-8.12	97.86	114.10
1	B	20	THR	N-CA-CB	-8.07	96.84	110.41
1	A	51	THR	CA-CB-CG2	8.03	124.16	110.50
1	B	188	GLY	O-C-N	-7.98	114.53	122.19
1	B	309	LYS	CA-C-N	7.98	131.31	120.54
1	B	309	LYS	C-N-CA	7.98	131.31	120.54
1	B	146	GLY	CA-C-N	7.89	131.64	120.28
1	B	146	GLY	C-N-CA	7.89	131.64	120.28
1	A	266	SER	CA-C-N	7.88	130.68	120.44
1	A	266	SER	C-N-CA	7.88	130.68	120.44
1	B	94	SER	N-CA-C	7.86	120.99	111.40
1	B	60	PHE	CA-C-N	7.85	134.03	120.68
1	B	60	PHE	C-N-CA	7.85	134.03	120.68
1	B	103	PHE	CA-CB-CG	7.85	121.65	113.80
1	A	19	TRP	CA-C-O	7.84	129.72	120.70
1	B	53	HIS	N-CA-CB	7.80	123.39	110.52
1	A	246	ASN	CA-C-N	7.74	127.57	121.61
1	A	246	ASN	C-N-CA	7.74	127.57	121.61
1	A	343	LEU	CA-C-N	7.70	133.98	120.74
1	A	343	LEU	C-N-CA	7.70	133.98	120.74
1	B	333	GLU	CA-CB-CG	7.69	129.47	114.10
1	A	215	PRO	CA-C-O	-7.63	112.36	121.67
1	B	131	GLU	CA-C-O	7.59	127.98	119.41
1	A	149	ASP	N-CA-CB	7.58	122.87	110.37
1	A	250	GLY	N-CA-C	7.57	121.39	111.70
1	A	201	PHE	CA-CB-CG	7.56	121.36	113.80
1	A	334	ALA	CA-C-N	7.54	130.72	120.54
1	A	334	ALA	C-N-CA	7.54	130.72	120.54
1	A	170	ASP	CA-C-O	-7.49	112.84	121.07
1	B	23	ASP	CB-CA-C	7.47	124.88	110.17
1	B	207	HIS	CA-C-N	7.46	129.53	120.13
1	B	207	HIS	C-N-CA	7.46	129.53	120.13
1	A	274	LEU	CA-C-N	7.44	132.93	120.88
1	A	274	LEU	C-N-CA	7.44	132.93	120.88
1	A	370	GLU	CA-C-O	-7.43	111.42	119.97
1	A	320	GLU	CA-C-N	7.41	130.22	120.28
1	A	320	GLU	C-N-CA	7.41	130.22	120.28
1	B	328	ASP	CA-C-O	7.41	126.77	119.51
1	B	209	ASP	CA-C-O	-7.41	111.90	120.20
1	B	20	THR	CA-CB-CG2	7.37	123.03	110.50
1	A	58	ILE	CA-C-O	7.36	124.84	119.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	SER	N-CA-C	7.36	120.17	111.71
1	A	67	ARG	NE-CZ-NH1	7.32	128.81	121.50
1	A	125	ALA	CA-C-N	7.30	129.94	120.44
1	A	125	ALA	C-N-CA	7.30	129.94	120.44
1	B	143	GLU	CA-C-O	7.28	127.64	119.41
1	A	187	ARG	NE-CZ-NH2	-7.26	112.67	119.20
1	B	14	LEU	CA-C-N	7.22	132.78	120.72
1	B	14	LEU	C-N-CA	7.22	132.78	120.72
1	A	14	LEU	CA-C-N	7.22	132.78	120.72
1	A	14	LEU	C-N-CA	7.22	132.78	120.72
1	B	391	LEU	CA-C-N	7.21	134.28	120.66
1	B	391	LEU	C-N-CA	7.21	134.28	120.66
1	A	96	PRO	CA-C-N	7.20	130.32	120.46
1	A	96	PRO	C-N-CA	7.20	130.32	120.46
1	A	221	GLN	CA-C-N	7.20	132.74	120.72
1	A	221	GLN	C-N-CA	7.20	132.74	120.72
1	A	95	HIS	CA-C-N	7.19	126.90	119.56
1	A	95	HIS	C-N-CA	7.19	126.90	119.56
1	B	387	ILE	N-CA-CB	7.19	118.96	110.55
1	A	263	ASP	CA-C-N	7.17	129.76	120.44
1	A	263	ASP	C-N-CA	7.17	129.76	120.44
1	A	270	THR	CA-C-N	7.17	129.59	120.56
1	A	270	THR	C-N-CA	7.17	129.59	120.56
1	A	389	HIS	CA-CB-CG	-7.16	106.64	113.80
1	A	341	PHE	CA-C-O	-7.16	112.83	120.42
1	B	149	ASP	N-CA-C	-7.15	95.97	108.20
1	A	308	ALA	CA-C-O	7.14	128.32	120.82
1	B	37	GLU	CA-CB-CG	7.08	128.25	114.10
1	B	319	LYS	CA-C-N	7.07	129.63	120.44
1	B	319	LYS	C-N-CA	7.07	129.63	120.44
1	A	59	PRO	CA-C-N	7.05	129.60	120.44
1	A	59	PRO	C-N-CA	7.05	129.60	120.44
1	B	37	GLU	CA-C-N	7.04	130.58	120.79
1	B	37	GLU	C-N-CA	7.04	130.58	120.79
1	B	40	HIS	CA-CB-CG	-7.03	106.77	113.80
1	B	137	GLY	CA-C-N	6.99	128.87	120.14
1	B	137	GLY	C-N-CA	6.99	128.87	120.14
1	B	367	PHE	CA-C-N	-6.98	113.14	122.85
1	B	367	PHE	C-N-CA	-6.98	113.14	122.85
1	A	302	ASP	CA-CB-CG	-6.97	105.63	112.60
1	B	34	ASP	CB-CA-C	6.94	119.46	109.26
1	B	244	ASP	CA-CB-CG	6.90	119.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	LEU	N-CA-C	6.87	118.42	111.07
1	A	235	LEU	CA-C-O	6.87	128.03	120.82
1	B	56	ASP	N-CA-C	-6.85	103.60	112.23
1	B	7	ALA	CA-C-N	6.85	132.16	120.72
1	B	7	ALA	C-N-CA	6.85	132.16	120.72
1	B	142	SER	O-C-N	6.83	130.12	123.29
1	A	372	ALA	CA-C-N	6.83	132.12	120.72
1	A	372	ALA	C-N-CA	6.83	132.12	120.72
1	B	320	GLU	CA-C-N	6.83	129.43	120.28
1	B	320	GLU	C-N-CA	6.83	129.43	120.28
1	B	346	THR	CA-CB-OG1	-6.82	99.37	109.60
1	B	297	ARG	CA-C-N	6.81	130.67	120.31
1	B	297	ARG	C-N-CA	6.81	130.67	120.31
1	A	174	ASN	CA-CB-CG	6.76	119.36	112.60
1	B	357	LEU	CA-C-N	6.76	129.66	120.54
1	B	357	LEU	C-N-CA	6.76	129.66	120.54
1	A	54	ASP	CA-C-O	-6.75	113.68	120.90
1	A	139	ARG	NE-CZ-NH1	6.74	128.24	121.50
1	B	208	GLY	CA-C-N	6.73	130.21	120.38
1	B	208	GLY	C-N-CA	6.73	130.21	120.38
1	A	40	HIS	CA-CB-CG	-6.69	107.11	113.80
1	A	5	THR	O-C-N	-6.68	116.05	121.80
1	A	143	GLU	CA-C-N	6.68	132.95	122.94
1	A	143	GLU	C-N-CA	6.68	132.95	122.94
1	A	359	ASN	CA-C-O	-6.68	111.46	119.27
1	B	76	GLN	CA-C-N	6.67	129.11	120.44
1	B	76	GLN	C-N-CA	6.67	129.11	120.44
1	A	12	PHE	CA-C-N	-6.66	114.39	121.45
1	A	12	PHE	C-N-CA	-6.66	114.39	121.45
1	A	332	GLN	CA-C-N	6.64	129.47	120.44
1	A	332	GLN	C-N-CA	6.64	129.47	120.44
1	B	376	ASN	CA-C-O	-6.64	113.48	120.58
1	B	235	LEU	CA-C-O	6.63	127.78	120.82
1	A	53	HIS	N-CA-CB	6.63	121.45	110.52
1	B	168	ILE	CA-C-N	6.62	129.05	120.44
1	B	168	ILE	C-N-CA	6.62	129.05	120.44
1	B	214	ASN	OD1-CG-ND2	-6.62	115.98	122.60
1	A	268	PHE	CA-C-O	-6.61	113.80	121.07
1	A	67	ARG	CD-NE-CZ	6.61	133.66	124.40
1	A	51	THR	CA-CB-OG1	-6.60	99.69	109.60
1	A	354	ALA	CA-C-N	6.58	129.42	120.54
1	A	354	ALA	C-N-CA	6.58	129.42	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	ALA	O-C-N	-6.58	114.52	122.22
1	A	256	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	280	ASN	CA-C-O	-6.57	111.33	119.28
1	B	188	GLY	CA-C-N	6.54	131.99	122.77
1	B	188	GLY	C-N-CA	6.54	131.99	122.77
1	A	391	LEU	CA-C-N	6.54	134.22	121.41
1	A	391	LEU	C-N-CA	6.54	134.22	121.41
1	B	343	LEU	CA-C-N	6.53	132.42	120.79
1	B	343	LEU	C-N-CA	6.53	132.42	120.79
1	B	390	LEU	O-C-N	-6.53	115.20	122.12
1	B	311	ASN	CA-C-N	6.50	129.52	120.29
1	B	311	ASN	C-N-CA	6.50	129.52	120.29
1	A	203	GLU	CA-C-N	6.48	132.53	122.49
1	A	203	GLU	C-N-CA	6.48	132.53	122.49
1	A	94	SER	CA-C-O	-6.47	114.03	120.70
1	B	265	THR	CA-C-N	6.46	128.93	120.28
1	B	265	THR	C-N-CA	6.46	128.93	120.28
1	A	235	LEU	CA-C-N	6.44	128.91	120.28
1	A	235	LEU	C-N-CA	6.44	128.91	120.28
1	B	246	ASN	CB-CG-ND2	6.42	126.03	116.40
1	A	19	TRP	CA-C-N	6.42	131.44	120.72
1	A	19	TRP	C-N-CA	6.42	131.44	120.72
1	A	112	ARG	CD-NE-CZ	6.41	133.37	124.40
1	B	359	ASN	CB-CA-C	6.38	121.97	109.72
1	B	241	PHE	CA-CB-CG	6.38	120.18	113.80
1	B	360	ASP	CA-CB-CG	6.38	118.98	112.60
1	B	162	ASP	CA-C-O	-6.38	113.66	120.42
1	B	20	THR	CB-CA-C	6.37	122.63	109.95
1	B	334	ALA	CA-C-N	6.36	128.81	120.28
1	B	334	ALA	C-N-CA	6.36	128.81	120.28
1	B	223	ALA	CA-C-N	6.36	132.25	120.87
1	B	223	ALA	C-N-CA	6.36	132.25	120.87
1	B	302	ASP	CA-C-O	-6.36	113.81	120.55
1	A	7	ALA	CA-C-O	6.35	127.28	120.10
1	A	297	ARG	O-C-N	-6.34	114.14	122.39
1	A	44	GLU	N-CA-CB	6.34	119.44	110.12
1	A	111	ARG	CA-C-N	6.33	129.04	120.44
1	A	111	ARG	C-N-CA	6.33	129.04	120.44
1	A	65	ALA	N-CA-C	-6.32	104.30	111.07
1	A	342	GLU	CB-CA-C	-6.32	98.93	110.63
1	B	54	ASP	O-C-N	-6.31	114.57	122.20
1	A	20	THR	N-CA-CB	-6.30	99.93	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	GLU	CB-CG-CD	6.27	123.25	112.60
1	B	383	ASN	O-C-N	-6.27	115.01	122.15
1	B	276	ASN	CA-C-O	-6.24	112.30	119.60
1	A	128	MET	O-C-N	-6.23	113.86	122.46
1	B	106	ASN	CA-C-N	6.23	130.21	121.24
1	B	106	ASN	C-N-CA	6.23	130.21	121.24
1	A	383	ASN	CA-CB-CG	-6.22	106.38	112.60
1	A	362	ALA	CA-C-N	6.22	132.61	121.66
1	A	362	ALA	C-N-CA	6.22	132.61	121.66
1	B	320	GLU	CA-CB-CG	6.20	126.50	114.10
1	A	143	GLU	CA-C-O	6.20	126.42	119.41
1	B	34	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	115	LEU	CB-CA-C	6.19	121.37	110.85
1	A	121	ASN	CA-CB-CG	-6.16	106.44	112.60
1	B	372	ALA	CA-C-N	6.14	130.43	120.60
1	B	372	ALA	C-N-CA	6.14	130.43	120.60
1	A	162	ASP	CA-C-O	-6.13	113.92	120.42
1	B	63	THR	CA-C-O	-6.13	114.89	121.94
1	B	335	MET	CA-C-N	6.12	128.76	120.44
1	B	335	MET	C-N-CA	6.12	128.76	120.44
1	A	281	GLY	CA-C-O	-6.09	117.36	122.29
1	A	207	HIS	CA-C-N	6.08	131.62	120.79
1	A	207	HIS	C-N-CA	6.08	131.62	120.79
1	A	76	GLN	O-C-N	6.06	128.32	122.07
1	B	19	TRP	N-CA-CB	6.06	119.04	109.71
1	A	316	LEU	CB-CA-C	6.05	120.37	110.88
1	B	125	ALA	CA-C-N	6.03	128.28	120.44
1	B	125	ALA	C-N-CA	6.03	128.28	120.44
1	B	336	LYS	CA-C-N	6.03	128.28	120.44
1	B	336	LYS	C-N-CA	6.03	128.28	120.44
1	A	394	ARG	NE-CZ-NH2	-6.02	113.78	119.20
1	B	102	GLY	O-C-N	6.00	125.21	121.85
1	A	213	LEU	CD1-CG-CD2	-6.00	97.60	110.80
1	B	138	GLY	N-CA-C	6.00	121.09	113.24
1	A	81	THR	CA-CB-OG1	-6.00	100.61	109.60
1	A	139	ARG	NE-CZ-NH2	-5.98	113.82	119.20
1	A	272	ASP	CA-C-N	5.98	128.21	120.44
1	A	272	ASP	C-N-CA	5.98	128.21	120.44
1	B	108	ARG	NE-CZ-NH1	5.97	127.47	121.50
1	A	168	ILE	CA-C-N	5.96	128.19	120.44
1	A	168	ILE	C-N-CA	5.96	128.19	120.44
1	A	117	LYS	CA-C-N	5.96	128.07	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	LYS	C-N-CA	5.96	128.07	120.56
1	A	170	ASP	N-CA-CB	5.96	118.88	109.82
1	B	36	VAL	CB-CA-C	5.95	120.43	112.22
1	B	162	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	333	GLU	CA-C-N	5.93	128.15	120.44
1	A	333	GLU	C-N-CA	5.93	128.15	120.44
1	A	39	VAL	CA-C-N	5.93	128.15	120.44
1	A	39	VAL	C-N-CA	5.93	128.15	120.44
1	A	84	LYS	O-C-N	-5.93	115.74	122.68
1	A	352	GLU	N-CA-C	-5.93	99.23	108.90
1	A	310	ALA	CA-C-O	-5.93	114.27	120.55
1	A	152	ALA	CA-C-O	-5.93	114.14	120.42
1	B	190	ILE	CA-C-O	-5.92	113.98	120.84
1	A	303	GLY	CA-C-N	5.89	127.98	120.56
1	A	303	GLY	C-N-CA	5.89	127.98	120.56
1	A	320	GLU	CA-CB-CG	5.89	125.87	114.10
1	B	56	ASP	N-CA-CB	5.88	119.36	110.30
1	B	188	GLY	CA-C-O	5.88	126.81	120.75
1	A	33	LEU	CA-C-O	-5.87	114.03	120.43
1	A	52	PHE	CA-C-N	5.86	131.39	122.65
1	A	52	PHE	C-N-CA	5.86	131.39	122.65
1	A	305	TRP	CA-C-N	5.86	128.06	120.44
1	A	305	TRP	C-N-CA	5.86	128.06	120.44
1	A	120	HIS	CA-CB-CG	-5.86	107.94	113.80
1	A	269	PHE	CA-C-N	5.86	128.40	120.44
1	A	269	PHE	C-N-CA	5.86	128.40	120.44
1	A	332	GLN	OE1-CD-NE2	-5.84	116.76	122.60
1	B	150	LEU	CB-CA-C	5.84	120.49	110.79
1	B	119	LEU	CA-C-N	5.84	128.10	120.28
1	B	119	LEU	C-N-CA	5.84	128.10	120.28
1	A	298	THR	CA-C-N	5.83	130.71	122.09
1	A	298	THR	C-N-CA	5.83	130.71	122.09
1	B	197	HIS	N-CA-CB	5.83	118.69	110.12
1	B	102	GLY	CA-C-N	5.83	128.67	120.28
1	B	102	GLY	C-N-CA	5.83	128.67	120.28
1	A	34	ASP	CA-C-N	5.82	125.69	119.28
1	A	34	ASP	C-N-CA	5.82	125.69	119.28
1	A	241	PHE	CA-CB-CG	5.80	119.61	113.80
1	A	65	ALA	CA-C-O	-5.80	114.73	120.82
1	B	355	ALA	CA-C-O	-5.80	114.40	120.55
1	B	302	ASP	CA-C-N	5.79	126.41	119.98
1	B	302	ASP	C-N-CA	5.79	126.41	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	HIS	CA-CB-CG	-5.78	108.02	113.80
1	A	76	GLN	CA-C-O	-5.78	114.76	120.82
1	A	370	GLU	CG-CD-OE2	5.77	131.67	118.40
1	B	33	LEU	CA-C-O	-5.77	114.14	120.43
1	B	376	ASN	OD1-CG-ND2	-5.75	116.85	122.60
1	B	233	GLN	OE1-CD-NE2	-5.75	116.85	122.60
1	A	303	GLY	O-C-N	-5.73	116.69	122.19
1	B	370	GLU	CA-C-O	-5.73	114.80	120.82
1	B	233	GLN	CB-CG-CD	5.73	122.34	112.60
1	A	6	PRO	O-C-N	-5.71	114.92	122.64
1	B	118	VAL	CA-C-O	-5.71	115.12	121.17
1	A	208	GLY	O-C-N	-5.71	116.23	122.68
1	A	149	ASP	N-CA-C	-5.70	98.45	108.20
1	B	142	SER	CA-C-O	-5.70	115.18	121.28
1	A	121	ASN	CA-C-N	5.70	128.27	120.46
1	A	121	ASN	C-N-CA	5.70	128.27	120.46
1	A	118	VAL	CA-C-O	-5.68	115.15	121.17
1	B	278	PHE	N-CA-C	5.68	117.22	110.07
1	B	286	THR	OG1-CB-CG2	5.66	120.62	109.30
1	A	40	HIS	CA-C-O	-5.66	114.88	120.82
1	A	138	GLY	N-CA-C	5.65	119.72	112.83
1	A	44	GLU	CA-CB-CG	5.64	125.38	114.10
1	B	162	ASP	CB-CA-C	5.64	120.43	110.85
1	B	44	GLU	CA-CB-CG	5.63	125.37	114.10
1	B	126	ALA	CA-C-N	5.63	127.82	120.28
1	B	126	ALA	C-N-CA	5.63	127.82	120.28
1	B	108	ARG	CD-NE-CZ	5.62	132.27	124.40
1	A	95	HIS	O-C-N	-5.61	115.14	121.43
1	A	304	VAL	CA-C-O	-5.61	115.22	121.17
1	A	234	ALA	CA-C-N	5.61	127.73	120.44
1	A	234	ALA	C-N-CA	5.61	127.73	120.44
1	B	141	GLY	CA-C-O	-5.61	117.04	120.91
1	B	36	VAL	CA-C-O	-5.60	114.91	120.85
1	B	208	GLY	O-C-N	-5.59	116.43	122.19
1	B	169	LYS	CA-C-O	-5.58	114.96	120.82
1	B	53	HIS	CA-C-O	-5.56	114.63	120.80
1	A	368	ASP	CA-C-N	5.55	127.66	120.44
1	A	368	ASP	C-N-CA	5.55	127.66	120.44
1	B	278	PHE	CA-C-N	5.54	125.90	119.47
1	B	278	PHE	C-N-CA	5.54	125.90	119.47
1	A	236	TRP	CA-C-O	-5.53	114.69	120.55
1	A	360	ASP	CA-C-N	5.53	129.95	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	ASP	C-N-CA	5.53	129.95	120.72
1	B	318	LEU	CA-C-N	5.51	127.67	120.28
1	B	318	LEU	C-N-CA	5.51	127.67	120.28
1	B	388	GLU	CA-C-N	5.50	127.93	120.44
1	B	388	GLU	C-N-CA	5.50	127.93	120.44
1	A	342	GLU	CA-C-O	-5.50	113.88	120.10
1	B	159	GLU	CA-CB-CG	5.50	125.10	114.10
1	B	334	ALA	O-C-N	-5.50	116.29	122.12
1	A	194	THR	CA-CB-CG2	5.49	119.83	110.50
1	B	195	VAL	CA-C-N	5.49	126.19	119.99
1	B	195	VAL	C-N-CA	5.49	126.19	119.99
1	B	383	ASN	CA-C-N	5.49	127.63	120.28
1	B	383	ASN	C-N-CA	5.49	127.63	120.28
1	A	23	ASP	CB-CA-C	5.48	120.97	110.17
1	A	99	LYS	CA-C-O	-5.48	113.90	120.10
1	A	60	PHE	CA-CB-CG	5.47	119.28	113.80
1	B	280	ASN	CA-C-O	-5.47	112.95	119.35
1	A	220	GLU	CA-C-N	5.45	129.83	120.72
1	A	220	GLU	C-N-CA	5.45	129.83	120.72
1	A	274	LEU	N-CA-C	5.45	117.22	111.28
1	A	370	GLU	CG-CD-OE1	-5.43	105.91	118.40
1	B	264	LEU	N-CA-C	5.43	117.20	111.28
1	A	55	ASN	CA-C-N	5.43	129.86	120.58
1	A	55	ASN	C-N-CA	5.43	129.86	120.58
1	A	14	LEU	O-C-N	-5.42	115.87	122.22
1	A	279	PRO	CA-C-N	5.42	132.20	122.38
1	A	279	PRO	C-N-CA	5.42	132.20	122.38
1	B	254	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	272	ASP	O-C-N	-5.41	116.50	122.07
1	B	365	ALA	CA-C-O	-5.40	114.80	120.63
1	B	184	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	B	379	PHE	CA-C-O	-5.36	113.81	119.97
1	A	206	GLU	N-CA-C	-5.35	105.36	111.14
1	A	270	THR	CA-CB-CG2	5.34	119.58	110.50
1	B	267	ALA	N-CA-CB	5.34	117.76	110.01
1	A	45	LEU	CA-C-O	-5.32	112.83	119.38
1	A	56	ASP	N-CA-CB	5.32	118.13	110.20
1	A	279	PRO	O-C-N	-5.32	116.44	122.18
1	B	165	ALA	CA-C-N	5.32	125.88	119.98
1	B	165	ALA	C-N-CA	5.32	125.88	119.98
1	B	196	GLY	CA-C-N	5.31	127.40	120.28
1	B	196	GLY	C-N-CA	5.31	127.40	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ASN	CB-CG-ND2	5.31	124.36	116.40
1	B	96	PRO	O-C-N	-5.31	115.75	122.17
1	B	90	THR	CA-CB-OG1	-5.28	101.68	109.60
1	A	35	PRO	CA-C-N	5.28	127.21	120.56
1	A	35	PRO	C-N-CA	5.28	127.21	120.56
1	A	214	ASN	CB-CG-ND2	5.27	124.30	116.40
1	B	384	GLN	CA-C-N	5.27	127.34	120.28
1	B	384	GLN	C-N-CA	5.27	127.34	120.28
1	B	249	ARG	O-C-N	-5.26	116.52	122.84
1	B	295	PRO	CB-CA-C	5.26	117.83	111.46
1	B	278	PHE	N-CA-CB	-5.26	103.19	110.29
1	B	34	ASP	CA-C-N	5.25	125.06	119.28
1	B	34	ASP	C-N-CA	5.25	125.06	119.28
1	B	351	GLY	CA-C-O	-5.25	114.00	119.20
1	B	96	PRO	CA-C-N	5.24	128.75	120.47
1	B	96	PRO	C-N-CA	5.24	128.75	120.47
1	B	215	PRO	N-CA-CB	5.24	107.91	103.35
1	A	265	THR	O-C-N	-5.24	116.68	122.07
1	A	75	ASN	CB-CG-ND2	5.23	124.25	116.40
1	B	67	ARG	CA-C-N	5.23	127.29	120.28
1	B	67	ARG	C-N-CA	5.23	127.29	120.28
1	B	36	VAL	CA-C-N	5.22	127.23	120.44
1	B	36	VAL	C-N-CA	5.22	127.23	120.44
1	B	305	TRP	CA-C-N	5.22	127.22	120.44
1	B	305	TRP	C-N-CA	5.22	127.22	120.44
1	A	83	LEU	CB-CA-C	5.21	118.56	109.65
1	A	105	SER	N-CA-C	-5.21	103.27	110.35
1	B	134	VAL	CA-C-N	5.21	130.25	122.86
1	B	134	VAL	C-N-CA	5.21	130.25	122.86
1	A	206	GLU	N-CA-CB	5.20	117.61	110.07
1	A	305	TRP	O-C-N	-5.20	115.88	122.27
1	A	316	LEU	CA-C-O	-5.19	115.37	120.82
1	A	32	ASN	CA-CB-CG	-5.19	107.41	112.60
1	B	45	LEU	CA-C-O	-5.19	112.87	119.31
1	B	44	GLU	N-CA-CB	5.19	118.21	110.22
1	B	127	GLU	CA-CB-CG	5.19	124.48	114.10
1	A	219	HIS	CA-C-O	-5.19	115.05	120.55
1	B	203	GLU	CG-CD-OE2	5.18	130.32	118.40
1	B	321	ARG	CA-CB-CG	-5.18	103.73	114.10
1	B	332	GLN	CA-C-N	5.18	127.18	120.44
1	B	332	GLN	C-N-CA	5.18	127.18	120.44
1	B	255	GLN	CA-C-N	5.17	129.69	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	GLN	C-N-CA	5.17	129.69	122.36
1	B	55	ASN	CB-CA-C	5.16	120.29	110.27
1	B	281	GLY	CA-C-O	-5.16	118.11	122.29
1	A	393	SER	N-CA-C	-5.16	106.39	113.30
1	B	246	ASN	CA-CB-CG	5.15	117.75	112.60
1	A	71	LEU	CA-C-N	5.15	125.65	119.94
1	A	71	LEU	C-N-CA	5.15	125.65	119.94
1	A	297	ARG	N-CA-C	5.13	118.64	112.38
1	B	333	GLU	CA-C-N	5.13	127.41	120.38
1	B	333	GLU	C-N-CA	5.13	127.41	120.38
1	B	32	ASN	CA-C-O	-5.13	116.11	121.55
1	A	208	GLY	CA-C-N	5.12	127.14	120.28
1	A	208	GLY	C-N-CA	5.12	127.14	120.28
1	A	359	ASN	N-CA-CB	5.12	118.43	110.44
1	A	167	TYR	CA-C-N	5.12	127.20	120.60
1	A	167	TYR	C-N-CA	5.12	127.20	120.60
1	A	236	TRP	N-CA-C	-5.12	105.70	111.28
1	A	106	ASN	N-CA-C	-5.11	105.79	111.36
1	A	58	ILE	N-CA-C	5.11	112.61	107.55
1	A	329	PRO	CB-CA-C	5.11	121.04	112.62
1	B	273	LEU	CA-CB-CG	5.08	134.07	116.30
1	B	64	GLU	CA-C-N	5.07	127.33	120.44
1	B	64	GLU	C-N-CA	5.07	127.33	120.44
1	A	84	LYS	CA-CB-CG	5.06	124.22	114.10
1	A	84	LYS	CA-C-N	5.06	131.49	122.13
1	A	84	LYS	C-N-CA	5.06	131.49	122.13
1	B	348	LEU	CA-C-O	-5.05	115.30	121.36
1	A	56	ASP	N-CA-C	-5.04	105.48	111.69
1	B	322	ALA	CA-C-N	5.04	127.29	120.44
1	B	322	ALA	C-N-CA	5.04	127.29	120.44
1	A	330	GLU	CA-C-N	5.04	127.57	120.42
1	A	330	GLU	C-N-CA	5.04	127.57	120.42
1	B	194	THR	CA-CB-CG2	5.04	119.06	110.50
1	B	375	ARG	NE-CZ-NH2	-5.04	114.67	119.20
1	B	53	HIS	N-CA-C	-5.03	101.50	109.76
1	A	20	THR	CA-CB-CG2	5.03	119.05	110.50
1	A	56	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	364	PHE	CA-C-N	5.03	128.36	120.82
1	A	364	PHE	C-N-CA	5.03	128.36	120.82
1	A	209	ASP	CA-C-O	-5.03	115.22	120.55
1	A	147	SER	CA-C-N	5.02	130.48	122.59
1	A	147	SER	C-N-CA	5.02	130.48	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	PHE	N-CA-CB	5.02	118.72	110.39
1	A	301	TYR	N-CA-C	5.01	121.47	110.80
1	B	231	ILE	CA-C-N	5.01	126.95	120.44
1	B	231	ILE	C-N-CA	5.01	126.95	120.44
1	B	14	LEU	O-C-N	-5.00	116.82	122.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	30	1
1	B	3027	0	2882	18	1
2	A	11	0	11	0	0
2	B	11	0	11	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	256	0	0	4	0
4	B	248	0	0	1	1
All	All	6584	0	5786	47	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 4.

All (47) 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:95:HIS:HD2	1:B:97:VAL:H	1.41	0.68
1:A:95:HIS:HD2	1:A:97:VAL:H	1.39	0.68
1:A:135:MET:HE1	1:A:161:VAL:HG22	1.79	0.65
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.79	0.64
1:A:23:ASP:HB2	1:A:24:PRO:HD2	1.80	0.62
1:A:69:LYS:HE2	1:A:73:ASP:OD2	2.00	0.62
1:A:59:PRO:HG2	1:A:62:ALA:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.86	0.57
1:B:23:ASP:HB2	1:B:24:PRO:HD2	1.88	0.55
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.88	0.54
1:B:55:ASN:HA	1:B:58:ILE:O	2.08	0.54
1:B:256:ASP:HB3	1:B:293:TYR:HA	1.91	0.53
1:A:95:HIS:CD2	1:A:97:VAL:H	2.23	0.52
1:A:20:THR:HG23	1:A:28:ALA:CB	2.40	0.52
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.93	0.51
1:B:20:THR:HG23	1:B:28:ALA:CB	2.41	0.50
1:B:354:ALA:O	1:B:358:MET:HG3	2.12	0.50
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.95	0.49
1:A:84:LYS:HD2	4:A:422:HOH:O	2.13	0.48
1:A:202:ILE:HG21	1:A:239:LYS:HE3	1.96	0.48
1:A:215:PRO:HG2	1:A:231:ILE:HG22	1.96	0.47
1:B:2:VAL:HG23	1:B:3:GLN:H	1.79	0.47
1:A:20:THR:HG23	1:A:28:ALA:HB2	1.96	0.46
1:A:135:MET:CE	1:A:161:VAL:HG22	2.44	0.46
1:A:185:GLU:HA	1:A:186:PRO:HA	1.75	0.45
1:A:58:ILE:HG21	1:A:67:ARG:HG3	1.99	0.45
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.82	0.45
1:A:135:MET:HE2	1:A:177:ILE:HG21	2.00	0.44
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.80	0.43
1:B:20:THR:HG22	4:B:563:HOH:O	2.17	0.43
1:A:135:MET:HE2	1:A:177:ILE:CG2	2.48	0.43
1:A:84:LYS:HB2	4:A:627:HOH:O	2.17	0.43
1:A:140:GLU:HG3	1:A:157:MET:HE1	2.01	0.43
1:A:217:THR:HA	1:A:227:PHE:CD1	2.55	0.42
1:A:179:LEU:HD22	4:A:442:HOH:O	2.20	0.41
1:A:275:GLU:HG3	1:A:319:LYS:HG3	2.01	0.41
1:A:273:LEU:HD21	1:A:278:PHE:CE1	2.55	0.41
1:A:384:GLN:NE2	1:B:261:HIS:NE2	2.67	0.41
1:B:23:ASP:CB	1:B:24:PRO:HD2	2.50	0.41
1:B:202:ILE:HG12	1:B:211:VAL:HG12	2.01	0.41
1:A:20:THR:HB	4:A:535:HOH:O	2.21	0.41
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.55	0.41
1:B:313:SER:O	1:B:317:LEU:HG	2.21	0.41
1:A:58:ILE:CG2	1:A:67:ARG:HG3	2.51	0.40
1:A:180:GLU:HA	1:A:181:PRO:HD3	1.88	0.40
1:B:34:ASP:HA	1:B:35:PRO:HD3	1.83	0.40
1:B:63:THR:HG23	1:B:66:GLU:OE2	2.21	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)
4:B:515:HOH:O	4:B:580:HOH:O[4_555]	1.92	0.28
1:A:69:LYS:NZ	1:B:276:ASN:O[6_665]	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%)	373 (95%)	17 (4%)	1 (0%)	36	55
1	B	391/394 (99%)	380 (97%)	9 (2%)	2 (0%)	24	43
All	All	782/788 (99%)	753 (96%)	26 (3%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

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

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%)	290 (95%)	15 (5%)	22	45
1	B	305/310 (98%)	294 (96%)	11 (4%)	31	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	610/620 (98%)	584 (96%)	26 (4%)	26	51

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
1	A	20	THR
1	A	69	LYS
1	A	84	LYS
1	A	90	THR
1	A	150	LEU
1	A	171	LYS
1	A	174	ASN
1	A	273	LEU
1	A	284	LYS
1	A	302	ASP
1	A	330	GLU
1	A	336	LYS
1	A	359	ASN
1	A	370	GLU
1	B	20	THR
1	B	34	ASP
1	B	37	GLU
1	B	41	LYS
1	B	61	ASP
1	B	131	GLU
1	B	149	ASP
1	B	176	ARG
1	B	213	LEU
1	B	273	LEU
1	B	286	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) 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

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Mol	Chain	Res	Type
1	A	384	GLN
1	B	95	HIS
1	B	359	ASN

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 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	DIG	B	400	3	11,11,11	2.51	5 (45%)	12,15,15	2.03	5 (41%)
2	DIG	A	400	3	11,11,11	1.94	4 (36%)	12,15,15	2.25	5 (41%)

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	DIG	B	400	3	-	0/4/20/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DIG	A	400	3	-	2/4/20/20	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	DIG	C2-N5	-5.00	1.40	1.48
2	B	400	DIG	C4-C5	-4.28	1.49	1.53
2	A	400	DIG	C3-C2	3.48	1.57	1.53
2	B	400	DIG	O4-C4	-3.09	1.35	1.43
2	A	400	DIG	O1-C1	-3.00	1.29	1.42
2	B	400	DIG	O1-C1	-2.61	1.31	1.42
2	B	400	DIG	C5-N5	-2.55	1.44	1.48
2	A	400	DIG	C5-N5	-2.49	1.44	1.48
2	A	400	DIG	C2-N5	-2.16	1.45	1.48

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	DIG	C1-C2-N5	4.37	119.18	111.47
2	A	400	DIG	O1-C1-C2	3.88	120.51	111.10
2	B	400	DIG	O6-C6-C5	3.75	120.17	111.10
2	B	400	DIG	C3-C4-C5	3.11	107.27	102.55
2	A	400	DIG	O6-C6-C5	3.07	118.53	111.10
2	B	400	DIG	O4-C4-C5	3.03	121.02	112.92
2	A	400	DIG	C3-C4-C5	2.81	106.81	102.55
2	B	400	DIG	O1-C1-C2	2.46	117.05	111.10
2	A	400	DIG	C1-C2-C3	-2.26	109.79	113.68
2	B	400	DIG	C6-C5-C4	2.14	117.37	113.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	DIG	N5-C5-C6-O6
2	A	400	DIG	C4-C5-C6-O6

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.