



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:34 PM UTC

PDB ID : 7XIM / pdb_00007xim
Title : PROTEIN ENGINEERING OF XYLOSE (GLUCOSE) ISOMERASE FROM ACTINOPLANES MISSOURIENSIS. 1. CRYSTALLOGRAPHY AND SITE-DIRECTED MUTAGENESIS OF METAL BINDING SITES
Authors : Janin, J.
Deposited on : 1992-04-03
Resolution : 2.40 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

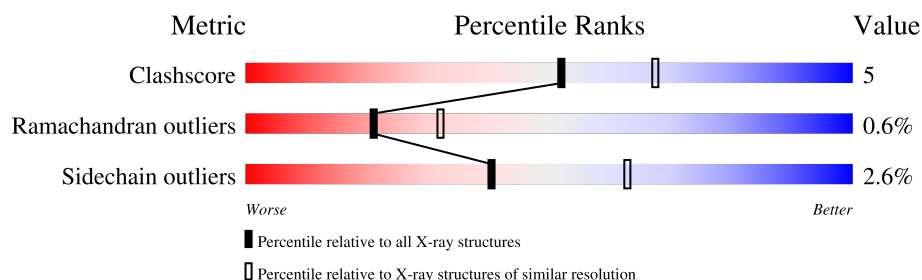
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	393	68% 25% 6% ..
1	B	393	67% 29% ..
1	C	393	72% 23% ..
1	D	393	67% 27% 5% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13067 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	390	Total	C	N	O	S	0	0	0
			3045	1933	531	577	4			
1	B	390	Total	C	N	O	S	0	0	0
			3045	1933	531	577	4			
1	C	390	Total	C	N	O	S	0	0	0
			3041	1931	530	576	4			
1	D	390	Total	C	N	O	S	0	0	0
			3041	1931	530	576	4			

- Molecule 2 is water.

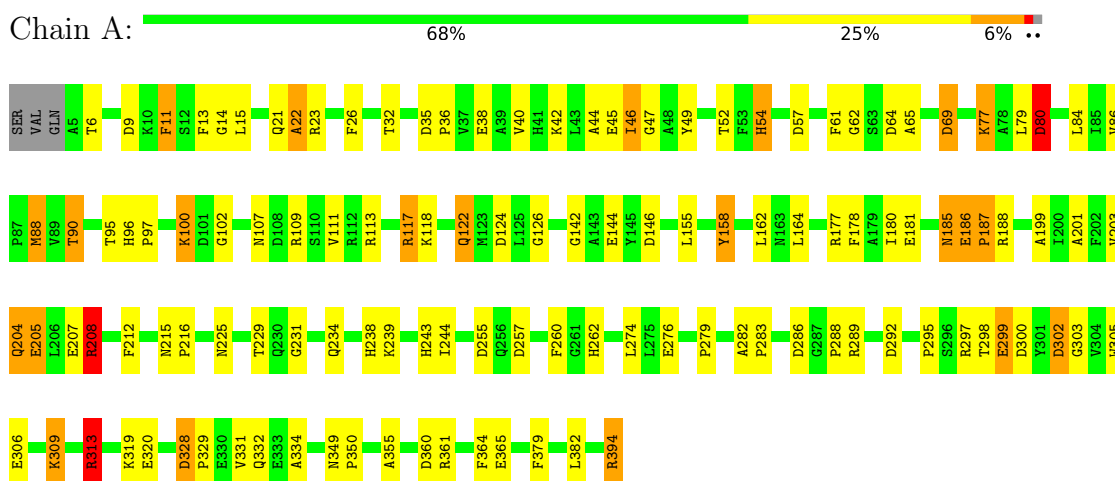
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	222	Total	O	0	0
			222	222		
2	B	218	Total	O	0	0
			218	218		
2	C	235	Total	O	0	0
			235	235		
2	D	220	Total	O	0	0
			220	220		

3 Residue-property plots

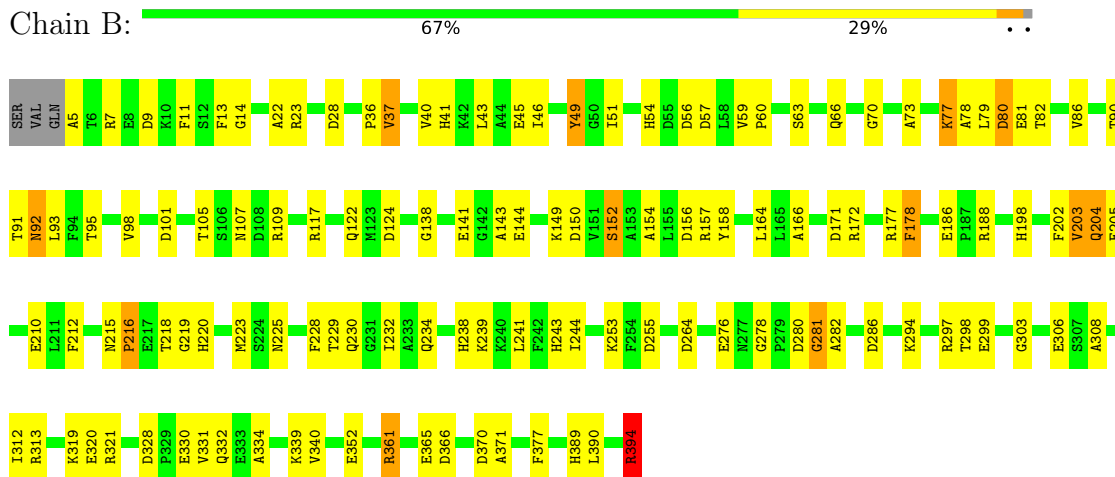
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

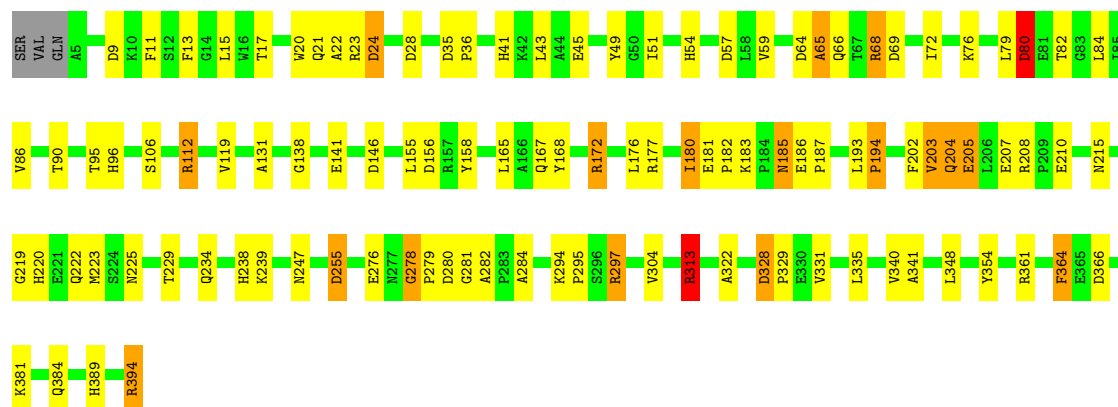


• Molecule 1: D-XYLOSE ISOMERASE



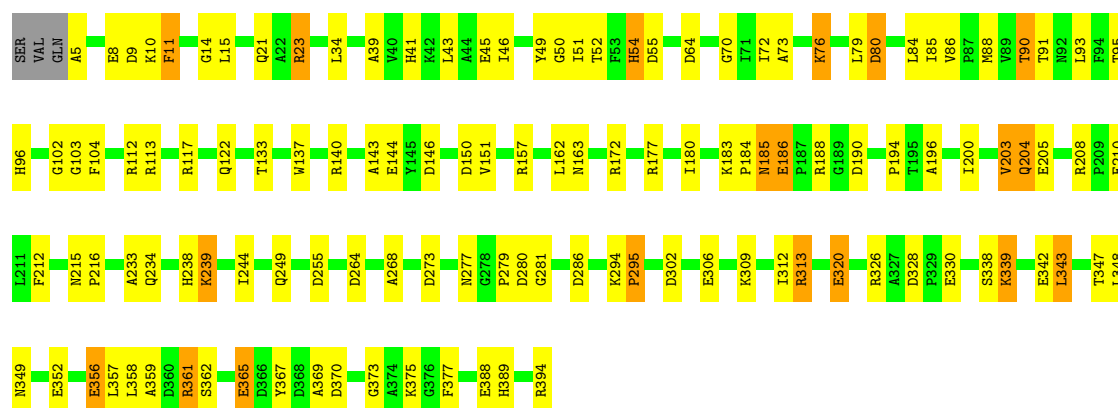
• Molecule 1: D-XYLOSE ISOMERASE





• Molecule 1: D-XYLOSE ISOMERASE

Chain D: 67% 27% 5% •



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.45Å 143.45Å 231.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.158 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13067	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.05	0/3117	2.17	126/4221 (3.0%)
1	B	1.03	0/3117	2.13	132/4221 (3.1%)
1	C	1.03	0/3113	2.07	104/4216 (2.5%)
1	D	1.03	1/3113 (0.0%)	2.15	128/4216 (3.0%)
All	All	1.04	1/12460 (0.0%)	2.13	490/16874 (2.9%)

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	C	0	2
1	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	103	GLY	N-CA	5.78	1.49	1.45

All (490) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ASP	CA-CB-CG	-18.55	94.05	112.60
1	B	204	GLN	OE1-CD-NE2	-17.30	105.30	122.60
1	D	204	GLN	OE1-CD-NE2	-14.89	107.71	122.60
1	C	204	GLN	OE1-CD-NE2	-13.73	108.86	122.60
1	D	80	ASP	CA-CB-CG	-12.25	100.35	112.60
1	A	394	ARG	CA-CB-CG	11.64	137.38	114.10
1	C	172	ARG	NE-CZ-NH1	11.60	133.10	121.50
1	D	172	ARG	CD-NE-CZ	11.43	140.39	124.40
1	A	107	ASN	CA-CB-CG	10.36	122.96	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	ARG	N-CA-CB	10.03	127.55	110.50
1	B	394	ARG	NE-CZ-NH2	-10.00	110.20	119.20
1	B	157	ARG	NE-CZ-NH1	9.96	131.46	121.50
1	A	204	GLN	OE1-CD-NE2	-9.91	112.69	122.60
1	B	23	ARG	CD-NE-CZ	9.87	138.22	124.40
1	D	328	ASP	CA-CB-CG	9.80	122.40	112.60
1	C	172	ARG	NE-CZ-NH2	-9.75	110.43	119.20
1	A	117	ARG	NE-CZ-NH1	9.62	131.12	121.50
1	A	225	ASN	OD1-CG-ND2	-9.08	113.52	122.60
1	B	77	LYS	O-C-N	9.04	131.38	122.07
1	A	180	ILE	N-CA-CB	8.87	120.20	110.53
1	D	367	TYR	O-C-N	8.77	133.22	123.22
1	B	13	PHE	CA-CB-CG	8.76	122.56	113.80
1	A	188	ARG	CD-NE-CZ	8.65	136.51	124.40
1	B	90	THR	CA-CB-OG1	-8.58	96.73	109.60
1	C	80	ASP	CA-CB-CG	-8.54	104.06	112.60
1	C	361	ARG	NE-CZ-NH2	8.50	126.85	119.20
1	D	326	ARG	NE-CZ-NH2	8.29	126.67	119.20
1	D	361	ARG	NE-CZ-NH2	8.28	126.65	119.20
1	D	10	LYS	CB-CA-C	-8.21	100.86	111.86
1	D	54	HIS	N-CA-C	-8.11	97.11	110.17
1	A	379	PHE	CA-CB-CG	8.06	121.86	113.80
1	C	203	VAL	N-CA-CB	-8.02	99.63	110.54
1	B	394	ARG	NH1-CZ-NH2	7.97	129.66	119.30
1	B	286	ASP	CA-C-O	-7.95	110.09	119.48
1	A	57	ASP	CA-CB-CG	7.94	120.54	112.60
1	B	141	GLU	CB-CG-CD	7.94	126.10	112.60
1	B	57	ASP	CA-CB-CG	7.86	120.46	112.60
1	B	117	ARG	NE-CZ-NH1	7.83	129.33	121.50
1	A	117	ARG	NE-CZ-NH2	-7.79	112.19	119.20
1	A	204	GLN	CB-CG-CD	7.77	125.81	112.60
1	C	168	TYR	CA-C-N	7.73	130.49	120.44
1	C	168	TYR	C-N-CA	7.73	130.49	120.44
1	A	319	LYS	CA-C-O	7.73	129.17	120.90
1	C	354	TYR	CA-C-O	-7.68	112.41	120.55
1	D	286	ASP	CA-CB-CG	-7.67	104.93	112.60
1	A	199	ALA	CB-CA-C	7.65	123.49	110.79
1	A	61	PHE	CA-C-O	-7.62	113.33	120.95
1	B	143	ALA	N-CA-CB	-7.58	98.83	111.57
1	D	95	THR	N-CA-C	7.55	119.30	111.14
1	A	46	ILE	CA-C-O	-7.55	109.80	119.39
1	A	313	ARG	CG-CD-NE	7.54	128.58	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	54	HIS	N-CA-C	-7.50	98.39	110.32
1	A	207	GLU	CG-CD-OE1	7.50	135.64	118.40
1	D	143	ALA	O-C-N	7.46	130.85	123.46
1	B	328	ASP	CA-CB-CG	7.44	120.04	112.60
1	B	157	ARG	NH1-CZ-NH2	-7.42	109.65	119.30
1	C	24	ASP	CA-CB-CG	7.39	119.99	112.60
1	A	286	ASP	CA-CB-CG	-7.36	105.24	112.60
1	A	394	ARG	NH1-CZ-NH2	7.34	128.85	119.30
1	D	188	ARG	NE-CZ-NH2	7.32	125.79	119.20
1	C	331	VAL	CB-CA-C	7.28	121.55	112.02
1	C	208	ARG	CD-NE-CZ	-7.26	114.23	124.40
1	D	157	ARG	NE-CZ-NH2	7.26	125.73	119.20
1	B	204	GLN	CB-CG-CD	7.25	124.92	112.60
1	C	158	TYR	N-CA-C	-7.25	103.46	111.36
1	C	185	ASN	O-C-N	7.20	130.49	123.29
1	C	167	GLN	OE1-CD-NE2	-7.19	115.41	122.60
1	D	163	ASN	CA-CB-CG	-7.19	105.41	112.60
1	C	41	HIS	CA-CB-CG	-7.15	106.65	113.80
1	D	295	PRO	CB-CA-C	7.15	120.11	111.46
1	B	389	HIS	CA-CB-CG	-7.11	106.69	113.80
1	C	328	ASP	CA-CB-CG	7.09	119.69	112.60
1	B	124	ASP	O-C-N	7.08	129.37	122.07
1	B	366	ASP	CA-CB-CG	7.08	119.68	112.60
1	C	138	GLY	CA-C-N	7.06	128.96	120.14
1	C	138	GLY	C-N-CA	7.06	128.96	120.14
1	A	180	ILE	CB-CA-C	-7.03	102.01	111.15
1	C	215	ASN	CA-CB-CG	-7.01	105.58	112.60
1	B	331	VAL	N-CA-C	-7.00	103.95	110.53
1	C	366	ASP	CA-CB-CG	7.00	119.60	112.60
1	A	185	ASN	OD1-CG-ND2	-6.98	115.62	122.60
1	A	229	THR	CA-CB-OG1	-6.93	99.20	109.60
1	B	80	ASP	CA-CB-CG	-6.93	105.67	112.60
1	A	177	ARG	CD-NE-CZ	6.89	134.04	124.40
1	D	286	ASP	CA-C-O	-6.87	111.38	119.48
1	D	347	THR	CA-C-O	6.83	127.85	119.79
1	D	144	GLU	N-CA-C	-6.83	105.23	113.97
1	A	360	ASP	CA-C-N	6.81	130.09	120.28
1	A	360	ASP	C-N-CA	6.81	130.09	120.28
1	D	313	ARG	N-CA-C	-6.79	103.80	111.07
1	C	340	VAL	CB-CA-C	6.78	120.56	111.88
1	D	79	LEU	CA-C-O	6.75	127.70	120.55
1	C	146	ASP	CA-C-O	-6.72	113.42	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	VAL	CA-C-N	6.71	126.31	119.19
1	B	86	VAL	C-N-CA	6.71	126.31	119.19
1	C	112	ARG	NE-CZ-NH2	6.71	125.24	119.20
1	A	244	ILE	CA-C-O	-6.71	113.72	120.90
1	C	79	LEU	CA-C-O	6.70	127.85	120.82
1	B	107	ASN	N-CA-C	-6.69	104.01	111.71
1	B	141	GLU	CA-C-O	-6.69	113.04	120.60
1	A	88	MET	CA-C-O	-6.66	113.53	120.99
1	D	239	LYS	CB-CA-C	-6.65	103.31	111.82
1	A	201	ALA	O-C-N	-6.63	115.24	122.07
1	B	220	HIS	CA-CB-CG	-6.62	107.18	113.80
1	C	394	ARG	CD-NE-CZ	-6.61	115.14	124.40
1	B	178	PHE	O-C-N	6.59	131.14	123.30
1	C	57	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	126	GLY	CA-C-N	6.58	129.09	120.28
1	A	126	GLY	C-N-CA	6.58	129.09	120.28
1	D	177	ARG	N-CA-C	-6.57	99.21	109.72
1	B	166	ALA	CA-C-N	6.56	128.97	120.44
1	B	166	ALA	C-N-CA	6.56	128.97	120.44
1	D	212	PHE	N-CA-C	6.54	119.56	108.90
1	B	390	LEU	CA-C-O	-6.54	113.62	120.55
1	C	304	VAL	CA-C-O	-6.53	114.25	121.17
1	B	394	ARG	CD-NE-CZ	-6.52	115.27	124.40
1	D	377	PHE	CA-C-O	-6.50	111.45	119.18
1	A	100	LYS	CA-C-O	-6.49	112.93	120.20
1	D	349	ASN	CA-CB-CG	-6.49	106.11	112.60
1	A	13	PHE	CA-C-O	-6.49	113.53	121.06
1	C	202	PHE	CA-C-N	6.49	129.34	120.46
1	C	202	PHE	C-N-CA	6.49	129.34	120.46
1	A	289	ARG	NH1-CZ-NH2	6.48	127.72	119.30
1	D	367	TYR	CA-C-O	-6.48	113.22	120.54
1	A	44	ALA	CA-C-O	6.46	127.61	120.63
1	C	185	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	A	306	GLU	CB-CA-C	-6.45	100.75	110.88
1	C	331	VAL	N-CA-C	-6.45	104.47	110.53
1	A	79	LEU	CA-C-O	6.44	127.38	120.55
1	A	42	LYS	CB-CA-C	-6.43	100.11	110.79
1	C	394	ARG	NE-CZ-NH1	-6.43	115.07	121.50
1	A	86	VAL	O-C-N	6.42	128.42	121.10
1	C	341	ALA	CA-C-O	-6.42	112.59	119.97
1	D	117	ARG	NE-CZ-NH1	6.41	127.91	121.50
1	D	76	LYS	O-C-N	6.41	128.91	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	PRO	CA-C-O	-6.40	113.86	121.67
1	D	90	THR	CA-CB-CG2	6.39	121.36	110.50
1	A	215	ASN	OD1-CG-ND2	-6.37	116.23	122.60
1	C	281	GLY	CA-C-N	6.36	130.35	120.68
1	C	281	GLY	C-N-CA	6.36	130.35	120.68
1	A	158	TYR	CA-C-N	6.35	128.70	120.44
1	A	158	TYR	C-N-CA	6.35	128.70	120.44
1	C	64	ASP	N-CA-C	-6.35	102.15	110.53
1	B	92	ASN	CA-CB-CG	-6.34	106.26	112.60
1	B	303	GLY	N-CA-C	-6.34	105.12	112.73
1	A	313	ARG	NE-CZ-NH1	-6.33	115.17	121.50
1	D	249	GLN	CA-CB-CG	6.33	126.75	114.10
1	C	45	GLU	CA-CB-CG	6.32	126.73	114.10
1	D	104	PHE	O-C-N	6.32	129.61	122.22
1	A	276	GLU	N-CA-C	6.30	121.21	112.45
1	B	91	THR	CA-C-O	-6.30	113.89	120.70
1	D	54	HIS	N-CA-CB	6.28	120.87	110.63
1	A	144	GLU	N-CA-CB	6.27	118.93	110.59
1	C	66	GLN	N-CA-C	-6.27	104.36	111.07
1	D	306	GLU	N-CA-C	-6.26	104.37	111.14
1	C	222	GLN	OE1-CD-NE2	-6.25	116.34	122.60
1	B	14	GLY	N-CA-C	-6.25	104.20	112.82
1	D	306	GLU	N-CA-CB	6.25	119.12	110.07
1	D	55	ASP	CA-CB-CG	6.21	118.81	112.60
1	C	96	HIS	CA-CB-CG	-6.21	107.59	113.80
1	D	10	LYS	O-C-N	6.21	130.03	122.58
1	C	95	THR	N-CA-C	6.20	117.91	111.03
1	D	163	ASN	O-C-N	6.20	128.69	122.12
1	D	349	ASN	OD1-CG-ND2	6.20	128.80	122.60
1	B	41	HIS	CA-CB-CG	-6.19	107.61	113.80
1	D	104	PHE	CA-C-O	-6.17	113.13	120.10
1	A	320	GLU	CB-CG-CD	6.15	123.06	112.60
1	B	313	ARG	CA-C-N	6.15	128.43	120.44
1	B	313	ARG	C-N-CA	6.15	128.43	120.44
1	B	54	HIS	CA-CB-CG	-6.14	107.66	113.80
1	B	366	ASP	CA-C-O	-6.13	112.71	119.95
1	D	264	ASP	CA-C-N	6.13	128.41	120.44
1	D	264	ASP	C-N-CA	6.13	128.41	120.44
1	B	57	ASP	N-CA-C	-6.13	104.15	111.69
1	D	277	ASN	OD1-CG-ND2	6.13	128.73	122.60
1	D	150	ASP	CA-CB-CG	-6.12	106.48	112.60
1	C	313	ARG	CA-CB-CG	6.11	126.32	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	GLY	CA-C-N	6.10	129.09	120.42
1	A	231	GLY	C-N-CA	6.10	129.09	120.42
1	C	194	PRO	N-CA-C	6.10	121.48	113.86
1	B	334	ALA	CA-C-O	-6.10	113.96	120.42
1	B	150	ASP	CA-CB-CG	-6.09	106.51	112.60
1	D	279	PRO	CA-C-O	6.08	127.97	121.03
1	A	26	PHE	CA-C-O	-6.08	112.00	119.18
1	D	326	ARG	CA-CB-CG	6.08	126.26	114.10
1	B	95	THR	N-CA-C	6.07	119.07	111.24
1	A	102	GLY	CA-C-O	-6.07	117.94	122.37
1	D	133	THR	CA-CB-OG1	-6.07	100.50	109.60
1	A	355	ALA	O-C-N	6.06	128.32	122.07
1	D	70	GLY	O-C-N	6.06	128.07	122.19
1	A	207	GLU	CG-CD-OE2	-6.05	104.48	118.40
1	B	171	ASP	CA-C-O	-6.04	114.02	120.42
1	B	340	VAL	CB-CA-C	6.04	119.61	111.88
1	C	229	THR	CA-CB-OG1	-6.04	100.54	109.60
1	D	96	HIS	CA-CB-CG	-6.03	107.77	113.80
1	B	328	ASP	CA-C-O	6.02	124.09	119.46
1	C	64	ASP	CA-CB-CG	-6.01	106.58	112.60
1	D	146	ASP	O-C-N	6.01	128.49	122.12
1	B	144	GLU	N-CA-C	-6.00	106.08	113.41
1	B	332	GLN	OE1-CD-NE2	-6.00	116.60	122.60
1	B	45	GLU	CA-CB-CG	5.99	126.07	114.10
1	A	21	GLN	CB-CG-CD	-5.98	102.43	112.60
1	B	321	ARG	NE-CZ-NH2	-5.98	113.82	119.20
1	A	54	HIS	N-CA-C	-5.98	100.54	110.17
1	B	54	HIS	N-CA-C	-5.98	100.54	110.17
1	C	28	ASP	CA-CB-CG	5.97	118.57	112.60
1	C	165	LEU	CA-C-O	-5.96	114.56	120.82
1	C	41	HIS	CA-C-O	-5.95	114.57	120.70
1	A	181	GLU	O-C-N	5.94	127.89	121.12
1	A	328	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	80	ASP	OD1-CG-OD2	5.92	137.11	122.90
1	A	177	ARG	N-CA-C	-5.92	100.54	109.95
1	A	13	PHE	O-C-N	5.92	130.13	123.27
1	B	122	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	C	165	LEU	O-C-N	5.91	128.15	122.07
1	B	218	THR	CA-CB-OG1	-5.90	100.75	109.60
1	C	54	HIS	N-CA-CB	5.90	120.02	110.41
1	B	253	LYS	CA-C-O	-5.89	115.01	121.31
1	B	361	ARG	CA-CB-CG	-5.88	102.33	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	370	ASP	CA-CB-CG	-5.87	106.73	112.60
1	D	151	VAL	N-CA-C	5.85	116.59	110.62
1	A	69	ASP	O-C-N	5.85	128.32	122.12
1	B	109	ARG	N-CA-C	5.85	118.43	111.71
1	A	274	LEU	CA-C-O	-5.83	114.70	120.82
1	C	278	GLY	CA-C-N	5.83	127.12	119.84
1	C	278	GLY	C-N-CA	5.83	127.12	119.84
1	B	73	ALA	CA-C-N	5.81	126.39	120.00
1	B	73	ALA	C-N-CA	5.81	126.39	120.00
1	D	194	PRO	N-CA-C	5.80	121.17	113.57
1	A	64	ASP	N-CA-C	-5.79	103.28	110.41
1	B	152	SER	CB-CA-C	5.79	119.97	110.88
1	B	281	GLY	CA-C-N	5.79	129.46	120.60
1	B	281	GLY	C-N-CA	5.79	129.46	120.60
1	B	215	ASN	CA-CB-CG	-5.79	106.81	112.60
1	A	295	PRO	N-CA-C	-5.78	102.08	110.80
1	C	13	PHE	CA-CB-CG	5.78	119.58	113.80
1	B	28	ASP	O-C-N	5.78	129.37	122.79
1	D	86	VAL	O-C-N	5.78	127.68	121.10
1	A	15	LEU	N-CA-CB	-5.77	101.33	110.22
1	A	298	THR	CA-CB-CG2	5.77	120.31	110.50
1	B	253	LYS	O-C-N	5.77	129.16	122.99
1	B	66	GLN	OE1-CD-NE2	5.76	128.36	122.60
1	D	80	ASP	O-C-N	5.75	127.99	122.07
1	A	286	ASP	CA-C-O	-5.75	112.48	119.32
1	B	204	GLN	CG-CD-OE1	5.75	132.29	120.80
1	A	289	ARG	NE-CZ-NH1	-5.74	115.76	121.50
1	D	306	GLU	CB-CA-C	-5.74	101.83	110.90
1	B	105	THR	CA-C-O	-5.73	113.01	119.95
1	A	146	ASP	CA-C-O	-5.73	114.48	120.55
1	D	342	GLU	CB-CG-CD	5.72	122.33	112.60
1	D	190	ASP	CA-C-O	-5.72	113.24	120.28
1	D	41	HIS	CA-CB-CG	-5.72	108.08	113.80
1	D	277	ASN	O-C-N	5.71	131.35	122.67
1	A	394	ARG	CD-NE-CZ	-5.71	116.41	124.40
1	B	45	GLU	CB-CG-CD	5.71	122.30	112.60
1	C	68	ARG	O-C-N	5.71	128.02	122.09
1	D	277	ASN	N-CA-C	-5.70	103.46	110.65
1	A	394	ARG	NE-CZ-NH2	-5.70	114.07	119.20
1	D	281	GLY	CA-C-N	5.70	130.14	121.03
1	D	281	GLY	C-N-CA	5.70	130.14	121.03
1	D	279	PRO	CB-CA-C	5.69	118.35	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	THR	CB-CA-C	5.69	120.44	111.39
1	A	302	ASP	CA-C-N	5.69	126.30	119.98
1	A	302	ASP	C-N-CA	5.69	126.30	119.98
1	B	330	GLU	OE1-CD-OE2	5.69	136.55	122.90
1	B	228	PHE	CA-C-O	-5.68	115.03	121.00
1	D	328	ASP	O-C-N	5.68	126.58	121.35
1	C	297	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	C	207	GLU	CG-CD-OE2	-5.67	105.36	118.40
1	C	23	ARG	N-CA-C	-5.67	99.29	108.41
1	A	90	THR	CA-CB-OG1	-5.66	101.10	109.60
1	C	155	LEU	CB-CA-C	5.66	120.19	110.79
1	C	225	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	D	88	MET	CA-CB-CG	5.65	125.41	114.10
1	A	109	ARG	NE-CZ-NH2	-5.65	114.12	119.20
1	C	177	ARG	N-CA-C	-5.64	100.50	109.59
1	D	302	ASP	O-C-N	5.63	128.09	122.12
1	B	177	ARG	NE-CZ-NH2	-5.62	114.14	119.20
1	B	202	PHE	CA-C-N	5.62	128.16	120.46
1	B	202	PHE	C-N-CA	5.62	128.16	120.46
1	D	45	GLU	CA-C-O	-5.61	113.77	120.10
1	D	313	ARG	CA-CB-CG	5.61	125.31	114.10
1	D	162	LEU	CA-C-N	5.59	127.78	120.28
1	D	162	LEU	C-N-CA	5.59	127.78	120.28
1	B	54	HIS	CB-CA-C	-5.59	100.06	109.50
1	D	203	VAL	CA-CB-CG1	5.59	119.89	110.40
1	C	80	ASP	N-CA-CB	-5.58	101.33	109.82
1	A	142	GLY	CA-C-O	-5.58	117.06	120.91
1	B	319	LYS	CA-C-N	5.58	127.75	120.28
1	B	319	LYS	C-N-CA	5.58	127.75	120.28
1	A	177	ARG	NE-CZ-NH1	5.57	127.07	121.50
1	B	370	ASP	CA-C-O	-5.57	114.65	120.55
1	A	155	LEU	CB-CA-C	5.56	120.30	110.85
1	A	262	HIS	N-CA-CB	5.55	118.94	110.44
1	D	320	GLU	CA-CB-CG	5.54	125.18	114.10
1	D	177	ARG	CD-NE-CZ	-5.53	116.66	124.40
1	A	124	ASP	CA-CB-CG	-5.53	107.07	112.60
1	D	358	LEU	CA-C-O	5.52	126.17	119.49
1	D	112	ARG	CD-NE-CZ	5.51	132.12	124.40
1	B	54	HIS	N-CA-CB	5.51	119.61	110.63
1	D	357	LEU	O-C-N	5.50	127.74	122.07
1	C	180	ILE	CA-CB-CG1	5.50	119.76	110.40
1	D	204	GLN	CB-CG-CD	5.50	121.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	CG-CD-NE	-5.50	99.91	112.00
1	D	369	ALA	CA-C-N	5.49	127.58	120.44
1	D	369	ALA	C-N-CA	5.49	127.58	120.44
1	C	335	LEU	O-C-N	5.49	127.94	122.12
1	D	268	ALA	N-CA-C	-5.49	105.30	111.28
1	C	204	GLN	CG-CD-OE1	5.48	131.77	120.80
1	D	309	LYS	CA-C-N	5.48	127.62	120.28
1	D	309	LYS	C-N-CA	5.48	127.62	120.28
1	C	247	ASN	OD1-CG-ND2	-5.47	117.12	122.60
1	D	309	LYS	CA-C-O	-5.47	114.75	120.55
1	C	79	LEU	CA-C-N	5.47	128.39	120.79
1	C	79	LEU	C-N-CA	5.47	128.39	120.79
1	D	122	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	A	69	ASP	CA-CB-CG	-5.46	107.14	112.60
1	A	118	LYS	CA-C-N	5.46	128.17	120.42
1	A	118	LYS	C-N-CA	5.46	128.17	120.42
1	B	138	GLY	CA-C-N	5.46	126.96	120.14
1	B	138	GLY	C-N-CA	5.46	126.96	120.14
1	B	243	HIS	CA-C-O	-5.45	115.60	121.38
1	C	119	VAL	CA-C-O	-5.45	115.00	121.05
1	B	218	THR	CA-CB-CG2	5.45	119.76	110.50
1	C	210	GLU	CB-CG-CD	5.45	121.86	112.60
1	D	302	ASP	CA-C-O	-5.45	114.78	120.55
1	B	308	ALA	CA-C-N	5.44	128.58	120.31
1	B	308	ALA	C-N-CA	5.44	128.58	120.31
1	D	273	ASP	CA-C-N	5.44	127.51	120.44
1	D	273	ASP	C-N-CA	5.44	127.51	120.44
1	C	141	GLU	CB-CG-CD	5.43	121.82	112.60
1	A	62	GLY	N-CA-C	5.42	123.43	115.08
1	C	177	ARG	CB-CA-C	5.42	119.14	109.38
1	B	210	GLU	CA-CB-CG	5.42	124.94	114.10
1	B	239	LYS	CA-CB-CG	-5.42	103.26	114.10
1	C	389	HIS	CA-CB-CG	-5.42	108.38	113.80
1	A	364	PHE	CA-C-N	5.42	127.85	120.54
1	A	364	PHE	C-N-CA	5.42	127.85	120.54
1	B	149	LYS	O-C-N	5.42	129.97	123.36
1	D	339	LYS	CB-CA-C	-5.42	102.95	111.51
1	B	225	ASN	CB-CG-ND2	5.42	124.52	116.40
1	C	281	GLY	CA-C-O	5.41	129.99	120.57
1	D	210	GLU	CB-CG-CD	5.41	121.80	112.60
1	A	205	GLU	CB-CG-CD	5.40	121.78	112.60
1	D	190	ASP	O-C-N	5.40	129.95	123.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	388	GLU	CG-CD-OE1	-5.40	105.98	118.40
1	B	244	ILE	CA-C-O	-5.39	115.13	120.90
1	B	366	ASP	O-C-N	5.39	128.89	122.26
1	C	205	GLU	CG-CD-OE2	5.39	130.79	118.40
1	D	361	ARG	NE-CZ-NH1	-5.38	116.11	121.50
1	A	350	PRO	CB-CA-C	5.38	118.42	111.64
1	D	23	ARG	N-CA-C	-5.38	99.75	108.41
1	D	86	VAL	CA-C-O	-5.38	112.74	119.95
1	D	215	ASN	CA-CB-CG	-5.38	107.22	112.60
1	B	70	GLY	CA-C-N	5.38	127.33	120.56
1	B	70	GLY	C-N-CA	5.38	127.33	120.56
1	C	328	ASP	CB-CA-C	5.37	118.11	109.41
1	B	299	GLU	N-CA-C	5.37	118.81	110.17
1	A	122	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	D	330	GLU	OE1-CD-OE2	5.36	135.76	122.90
1	C	90	THR	CA-CB-OG1	-5.35	101.57	109.60
1	B	158	TYR	CA-C-O	5.35	126.21	120.70
1	A	146	ASP	N-CA-C	5.35	117.11	111.28
1	A	144	GLU	N-CA-C	-5.35	107.30	113.88
1	B	229	THR	CA-CB-OG1	-5.34	101.58	109.60
1	D	239	LYS	CA-C-O	-5.34	115.04	121.40
1	B	320	GLU	CB-CG-CD	5.34	121.68	112.60
1	B	339	LYS	CA-CB-CG	-5.34	103.42	114.10
1	B	82	THR	CA-C-O	-5.34	113.49	119.79
1	B	243	HIS	CA-CB-CG	5.34	119.14	113.80
1	C	328	ASP	CA-C-N	5.34	125.66	119.47
1	C	328	ASP	C-N-CA	5.34	125.66	119.47
1	D	389	HIS	CA-CB-CG	-5.33	108.47	113.80
1	C	384	GLN	CA-C-O	-5.33	114.90	120.55
1	B	230	GLN	CA-C-O	-5.33	114.90	120.55
1	B	93	LEU	CA-C-N	-5.32	113.94	122.08
1	B	93	LEU	C-N-CA	-5.32	113.94	122.08
1	A	288	PRO	CA-C-N	5.32	131.58	123.23
1	A	288	PRO	C-N-CA	5.32	131.58	123.23
1	B	158	TYR	N-CA-C	-5.31	105.40	111.14
1	C	281	GLY	N-CA-C	-5.31	100.59	113.18
1	A	255	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	255	ASP	CB-CA-C	5.31	118.74	110.67
1	C	66	GLN	N-CA-CB	5.31	117.70	110.01
1	B	37	VAL	O-C-N	5.30	127.29	121.83
1	B	188	ARG	CD-NE-CZ	5.30	131.82	124.40
1	D	208	ARG	O-C-N	5.30	126.06	121.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	GLY	N-CA-C	-5.30	103.05	112.54
1	B	352	GLU	CA-C-O	-5.30	115.01	121.05
1	D	203	VAL	CB-CA-C	5.30	118.98	112.04
1	B	77	LYS	CA-C-O	-5.29	115.26	120.82
1	A	260	PHE	CA-CB-CG	-5.29	108.51	113.80
1	B	90	THR	CA-C-O	-5.29	115.59	121.51
1	B	339	LYS	CB-CA-C	-5.29	103.16	111.51
1	C	276	GLU	CG-CD-OE2	5.29	130.56	118.40
1	A	88	MET	O-C-N	5.28	129.30	123.33
1	D	342	GLU	CG-CD-OE2	5.27	130.52	118.40
1	D	113	ARG	NE-CZ-NH1	5.27	126.77	121.50
1	A	95	THR	CA-C-O	-5.26	114.92	120.55
1	A	95	THR	N-CA-C	5.26	117.81	111.40
1	D	328	ASP	CB-CA-C	5.25	116.95	109.38
1	B	63	SER	O-C-N	5.25	129.33	123.19
1	A	243	HIS	CA-CB-CG	5.25	119.05	113.80
1	D	356	GLU	CG-CD-OE2	5.25	130.47	118.40
1	A	243	HIS	CA-C-N	-5.25	114.02	122.25
1	A	243	HIS	C-N-CA	-5.25	114.02	122.25
1	C	82	THR	CA-CB-OG1	-5.24	101.73	109.60
1	A	349	ASN	OD1-CG-ND2	5.23	127.83	122.60
1	B	79	LEU	CA-C-N	5.23	128.06	120.79
1	B	79	LEU	C-N-CA	5.23	128.06	120.79
1	D	21	GLN	CB-CG-CD	-5.23	103.71	112.60
1	C	23	ARG	CD-NE-CZ	5.23	131.72	124.40
1	A	331	VAL	N-CA-C	-5.22	105.44	110.72
1	B	143	ALA	CA-C-O	-5.22	115.69	121.28
1	C	176	LEU	CA-C-N	5.22	130.50	122.93
1	C	176	LEU	C-N-CA	5.22	130.50	122.93
1	A	257	ASP	CA-C-O	-5.22	115.55	121.65
1	D	15	LEU	N-CA-CB	-5.22	102.19	110.22
1	A	334	ALA	CA-C-O	-5.21	114.89	120.42
1	A	309	LYS	CB-CA-C	-5.21	102.00	110.85
1	A	187	PRO	N-CA-C	5.21	125.64	112.10
1	C	156	ASP	O-C-N	5.20	127.43	122.07
1	B	198	HIS	CE1-NE2-CD2	-5.20	103.80	109.00
1	D	233	ALA	N-CA-CB	5.19	117.54	110.01
1	C	180	ILE	N-CA-CB	5.19	116.19	110.53
1	D	52	THR	CA-CB-OG1	-5.19	101.81	109.60
1	C	57	ASP	CA-C-O	-5.19	113.67	119.79
1	D	216	PRO	CA-C-O	-5.19	115.34	121.67
1	D	203	VAL	N-CA-CB	-5.18	103.99	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	VAL	CA-C-O	-5.18	115.36	120.85
1	B	377	PHE	CA-C-O	-5.18	113.25	119.15
1	D	93	LEU	CA-C-O	-5.18	114.28	120.65
1	B	276	GLU	CG-CD-OE2	5.17	130.28	118.40
1	A	47	GLY	N-CA-C	5.16	122.43	115.00
1	B	93	LEU	O-C-N	5.16	129.12	122.20
1	D	244	ILE	CA-C-O	-5.16	115.38	120.90
1	D	255	ASP	CA-CB-CG	5.15	117.75	112.60
1	C	66	GLN	O-C-N	5.14	127.36	122.07
1	D	239	LYS	O-C-N	5.14	128.48	122.67
1	B	23	ARG	N-CA-C	-5.13	100.15	108.41
1	B	264	ASP	CA-C-O	-5.13	115.83	121.58
1	B	255	ASP	N-CA-CB	-5.13	101.82	110.49
1	B	177	ARG	CB-CG-CD	-5.13	99.51	111.30
1	C	21	GLN	CB-CG-CD	-5.12	103.89	112.60
1	D	14	GLY	N-CA-C	-5.12	103.37	112.54
1	D	365	GLU	O-C-N	5.12	127.42	122.09
1	D	215	ASN	CB-CG-ND2	5.12	124.08	116.40
1	D	375	LYS	CA-C-N	5.12	125.77	120.60
1	D	375	LYS	C-N-CA	5.12	125.77	120.60
1	A	11	PHE	CA-C-O	-5.12	114.76	120.54
1	D	196	ALA	CA-C-N	5.12	125.62	119.94
1	D	196	ALA	C-N-CA	5.12	125.62	119.94
1	A	244	ILE	O-C-N	5.11	129.02	123.09
1	D	200	ILE	N-CA-CB	5.11	116.53	110.55
1	C	57	ASP	N-CA-C	-5.10	105.80	112.23
1	B	156	ASP	O-C-N	5.09	127.32	122.07
1	A	23	ARG	CA-C-O	-5.09	115.62	120.92
1	A	276	GLU	CG-CD-OE2	5.09	130.10	118.40
1	B	80	ASP	O-C-N	5.08	127.52	122.08
1	A	45	GLU	O-C-N	5.08	127.31	122.07
1	D	73	ALA	O-C-N	5.08	127.94	122.15
1	D	343	LEU	N-CA-C	-5.08	106.60	112.89
1	D	93	LEU	N-CA-C	-5.07	104.72	111.87
1	A	77	LYS	O-C-N	5.07	127.29	122.07
1	A	208	ARG	CB-CG-CD	5.07	122.96	111.30
1	A	216	PRO	CA-C-O	-5.07	115.49	121.67
1	B	198	HIS	ND1-CE1-NE2	5.07	113.47	108.40
1	C	207	GLU	CB-CA-C	5.06	118.83	110.88
1	A	299	GLU	O-C-N	5.06	128.75	123.03
1	A	382	LEU	N-CA-C	-5.05	105.77	111.28
1	A	332	GLN	N-CA-CB	5.05	117.54	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	23	ARG	CA-C-O	-5.05	115.18	120.58
1	C	187	PRO	N-CA-C	5.05	125.22	112.10
1	C	322	ALA	N-CA-C	-5.05	105.86	111.36
1	B	117	ARG	NE-CZ-NH2	-5.05	114.66	119.20
1	A	113	ARG	NE-CZ-NH2	-5.04	114.66	119.20
1	B	13	PHE	CA-C-O	-5.04	115.21	121.06
1	C	255	ASP	CA-C-O	-5.04	114.62	120.62
1	B	371	ALA	CA-C-O	-5.04	115.08	120.42
1	B	56	ASP	CA-C-O	-5.03	112.76	119.10
1	D	64	ASP	N-CA-C	-5.03	103.89	110.53
1	A	32	THR	O-C-N	5.03	128.83	122.65
1	C	180	ILE	CA-C-O	5.03	126.58	120.85
1	A	22	ALA	N-CA-C	5.02	118.65	111.92
1	B	361	ARG	CD-NE-CZ	-5.02	117.37	124.40
1	C	284	ALA	N-CA-C	-5.02	107.00	113.23
1	D	11	PHE	CA-CB-CG	5.01	118.81	113.80
1	A	292	ASP	CA-CB-CG	5.01	117.61	112.60
1	C	65	ALA	O-C-N	5.00	127.43	122.12
1	C	112	ARG	CA-C-O	-5.00	115.57	120.82

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	172	ARG	Sidechain
1	C	313	ARG	Sidechain
1	D	313	ARG	Sidechain

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	3045	0	2949	35	0
1	B	3045	0	2949	35	0
1	C	3041	0	2943	34	0
1	D	3041	0	2943	32	0
2	A	222	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	218	0	0	1	0
2	C	235	0	0	1	0
2	D	220	0	0	3	0
All	All	13067	0	11784	122	0

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 (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLN:OE1	1:C:204:GLN:OE1	1.72	1.08
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.72	1.04
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.13	0.93
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.18	0.88
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.20	0.86
1:A:36:PRO:O	1:A:40:VAL:HG23	1.77	0.83
1:B:77:LYS:O	1:B:80:ASP:HB2	1.81	0.81
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.28	0.79
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.09	0.67
1:D:43:LEU:HD12	1:D:51:ILE:HD12	1.79	0.64
1:A:6:THR:O	1:A:9:ASP:HB2	1.97	0.64
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.79	0.64
1:D:72:ILE:O	1:D:76:LYS:HG3	1.97	0.63
1:D:34:LEU:HD21	1:D:39:ALA:HB2	1.80	0.63
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.82	0.63
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.06	0.61
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.84	0.61
1:A:204:GLN:HG2	2:A:545:HOH:O	2.00	0.60
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.84	0.60
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.01	0.60
1:D:394:ARG:HD2	2:D:606:HOH:O	2.05	0.56
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.89	0.55
1:B:37:VAL:HG13	1:B:78:ALA:HB2	1.89	0.54
1:A:204:GLN:HB3	2:A:544:HOH:O	2.06	0.54
1:D:34:LEU:CD2	1:D:39:ALA:HB2	2.37	0.54
1:C:24:ASP:O	1:D:23:ARG:NH2	2.41	0.54
1:B:7:ARG:HG2	1:B:49:TYR:HB2	1.91	0.53
1:A:208:ARG:HB3	1:A:208:ARG:NH1	2.24	0.53
1:A:299:GLU:HB3	1:A:303:GLY:HA3	1.91	0.52
1:B:152:SER:HB2	2:D:567:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ALA:HB1	1:B:297:ARG:HG3	1.91	0.52
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.45	0.51
1:C:183:LYS:HE2	1:C:185:ASN:O	2.11	0.51
1:A:77:LYS:O	1:A:80:ASP:CB	2.59	0.51
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.92	0.51
1:C:43:LEU:HD12	1:C:51:ILE:HD12	1.94	0.50
1:C:59:VAL:HG21	1:C:68:ARG:HG3	1.92	0.50
1:C:278:GLY:HA3	1:C:282:ALA:O	2.12	0.49
1:D:54:HIS:CD2	1:D:90:THR:HG23	2.47	0.49
1:B:92:ASN:OD1	1:B:92:ASN:C	2.54	0.49
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.95	0.49
1:D:137:TRP:HB3	2:D:474:HOH:O	2.13	0.49
1:D:361:ARG:HB3	1:D:365:GLU:HB2	1.95	0.49
1:C:255:ASP:OD2	2:C:619:HOH:O	2.20	0.49
1:A:52:THR:HG21	1:A:88:MET:HE3	1.95	0.47
1:A:238:HIS:O	1:A:239:LYS:HB2	2.13	0.47
1:A:279:PRO:HG2	2:A:506:HOH:O	2.14	0.47
1:B:278:GLY:HA3	1:B:282:ALA:O	2.13	0.47
1:D:11:PHE:CE2	1:D:312:ILE:HG23	2.49	0.47
1:A:65:ALA:O	1:A:69:ASP:HB2	2.13	0.47
1:B:5:ALA:HB2	1:B:312:ILE:HG21	1.97	0.47
1:B:43:LEU:HD12	1:B:51:ILE:HD12	1.97	0.47
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.96	0.47
1:A:77:LYS:O	1:A:80:ASP:HB2	2.15	0.46
1:C:65:ALA:O	1:C:69:ASP:HB2	2.14	0.46
1:B:278:GLY:CA	1:B:282:ALA:O	2.63	0.46
1:A:164:LEU:HD12	1:C:348:LEU:HD11	1.96	0.46
1:A:305:TRP:O	1:A:309:LYS:HG3	2.15	0.46
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.98	0.46
1:D:5:ALA:HB2	1:D:312:ILE:HG21	1.98	0.46
1:B:361:ARG:HA	1:B:365:GLU:OE1	2.16	0.46
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.82	0.45
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.98	0.45
1:C:394:ARG:HH11	1:C:394:ARG:HD3	1.45	0.45
1:A:117:ARG:HG3	1:C:364:PHE:HB2	1.97	0.45
1:B:101:ASP:CG	1:B:101:ASP:O	2.59	0.45
1:A:186:GLU:HA	1:A:187:PRO:HA	1.68	0.44
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.52	0.44
1:C:328:ASP:HA	1:C:329:PRO:HD3	1.81	0.44
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.51	0.44
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ILE:O	1:C:76:LYS:HG3	2.18	0.44
1:B:394:ARG:HH11	1:B:394:ARG:HD3	1.63	0.44
1:C:9:ASP:HB3	1:C:11:PHE:CE2	2.53	0.44
1:B:280:ASP:C	1:B:282:ALA:H	2.25	0.43
1:A:178:PHE:HB2	1:A:212:PHE:CD1	2.54	0.43
1:B:98:VAL:HA	1:D:373:GLY:HA2	1.99	0.43
1:D:238:HIS:O	1:D:239:LYS:HB2	2.17	0.43
1:B:216:PRO:HG2	1:B:232:ILE:CD1	2.49	0.43
1:D:8:GLU:HG2	1:D:8:GLU:O	2.17	0.43
1:D:361:ARG:HH11	1:D:361:ARG:HD3	1.68	0.43
1:B:241:LEU:HD12	1:B:241:LEU:HA	1.93	0.43
1:B:294:LYS:HE2	2:B:583:HOH:O	2.19	0.43
1:C:76:LYS:O	1:C:80:ASP:HB2	2.19	0.43
1:C:86:VAL:O	1:C:131:ALA:HA	2.19	0.43
1:D:356:GLU:O	1:D:359:ALA:HB3	2.19	0.43
1:A:35:ASP:HA	1:A:36:PRO:HD3	1.83	0.42
1:D:102:GLY:HA2	1:D:140:ARG:HB2	2.01	0.42
1:B:9:ASP:HB3	1:B:11:PHE:CE2	2.54	0.42
1:C:15:LEU:HD13	1:C:51:ILE:HD11	2.01	0.42
1:A:122:GLN:O	1:A:122:GLN:HG3	2.19	0.42
1:A:313:ARG:C	1:A:313:ARG:HD3	2.42	0.42
1:B:178:PHE:HB2	1:B:212:PHE:CD2	2.55	0.42
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.19	0.42
1:B:36:PRO:O	1:B:40:VAL:HG23	2.19	0.42
1:C:297:ARG:HH11	1:C:297:ARG:HD3	1.67	0.42
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.80	0.42
1:C:294:LYS:HA	1:C:295:PRO:HD3	1.91	0.42
1:D:294:LYS:HA	1:D:295:PRO:HD3	1.87	0.42
1:D:50:GLY:HA2	1:D:85:ILE:O	2.20	0.42
1:B:219:GLY:O	1:B:223:MET:HG3	2.20	0.42
1:C:234:GLN:HE21	1:C:238:HIS:CE1	2.12	0.42
1:D:338:SER:O	1:D:339:LYS:HB2	2.20	0.41
1:A:313:ARG:CG	1:A:313:ARG:HH11	2.33	0.41
1:C:106:SER:O	1:C:112:ARG:HD3	2.20	0.41
1:D:185:ASN:HD22	1:D:186:GLU:HB2	1.84	0.41
1:A:100:LYS:HD2	1:B:298:THR:HA	2.03	0.41
1:B:164:LEU:C	1:B:164:LEU:HD23	2.45	0.41
1:C:183:LYS:HG3	1:C:220:HIS:CG	2.56	0.41
1:C:193:LEU:N	1:C:194:PRO:HD3	2.36	0.41
1:C:278:GLY:CA	1:C:282:ALA:O	2.68	0.41
1:C:181:GLU:HA	1:C:182:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:HIS:O	1:C:239:LYS:HB2	2.21	0.41
1:D:9:ASP:HB3	1:D:11:PHE:CE2	2.56	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.90	0.41
1:A:300:ASP:OD1	1:A:302:ASP:HB2	2.20	0.41
1:C:219:GLY:O	1:C:223:MET:HG3	2.21	0.41
1:A:158:TYR:O	1:A:162:LEU:HG	2.21	0.40
1:B:216:PRO:HG2	1:B:232:ILE:HD11	2.03	0.40
1:D:183:LYS:HG2	1:D:184:PRO:HD2	2.03	0.40
1:B:59:VAL:HA	1:B:60:PRO:HD3	1.96	0.40
1:B:203:VAL:HG22	1:B:212:PHE:HB3	2.03	0.40

There are no symmetry-related clashes.

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	388/393 (99%)	376 (97%)	11 (3%)	1 (0%)	36	50
1	B	388/393 (99%)	375 (97%)	11 (3%)	2 (0%)	24	37
1	C	388/393 (99%)	372 (96%)	12 (3%)	4 (1%)	12	20
1	D	388/393 (99%)	373 (96%)	13 (3%)	2 (0%)	24	37
All	All	1552/1572 (99%)	1496 (96%)	47 (3%)	9 (1%)	21	32

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	280	ASP
1	A	186	GLU
1	B	186	GLU
1	C	186	GLU
1	C	279	PRO

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Mol	Chain	Res	Type
1	C	364	PHE
1	D	186	GLU
1	D	280	ASP
1	B	281	GLY

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	306/310 (99%)	296 (97%)	10 (3%)	33	55
1	B	306/310 (99%)	300 (98%)	6 (2%)	48	70
1	C	305/310 (98%)	299 (98%)	6 (2%)	48	70
1	D	305/310 (98%)	295 (97%)	10 (3%)	33	55
All	All	1222/1240 (98%)	1190 (97%)	32 (3%)	40	63

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	46	ILE
1	A	49	TYR
1	A	80	ASP
1	A	84	LEU
1	A	185	ASN
1	A	203	VAL
1	A	208	ARG
1	A	313	ARG
1	A	394	ARG
1	B	46	ILE
1	B	49	TYR
1	B	81	GLU
1	B	172	ARG
1	B	203	VAL
1	B	394	ARG
1	C	49	TYR

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Mol	Chain	Res	Type
1	C	80	ASP
1	C	84	LEU
1	C	180	ILE
1	C	203	VAL
1	C	313	ARG
1	D	46	ILE
1	D	49	TYR
1	D	80	ASP
1	D	84	LEU
1	D	91	THR
1	D	180	ILE
1	D	185	ASN
1	D	203	VAL
1	D	320	GLU
1	D	362	SER

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	204	GLN
1	A	222	GLN
1	A	238	HIS
1	B	66	GLN
1	B	204	GLN
1	B	222	GLN
1	B	230	GLN
1	B	238	HIS
1	B	256	GLN
1	C	222	GLN
1	C	238	HIS
1	D	185	ASN
1	D	222	GLN
1	D	238	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.