



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:43 AM UTC

PDB ID : 2PFK / pdb_00002pfk
Title : THE CRYSTAL STRUCTURE OF UNLIGANDED PHOSPHOFRUCTOKINASE FROM ESCHERICHIA COLI
Authors : Rypniewski, W.R.; Evans, P.R.
Deposited on : 1988-01-25
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

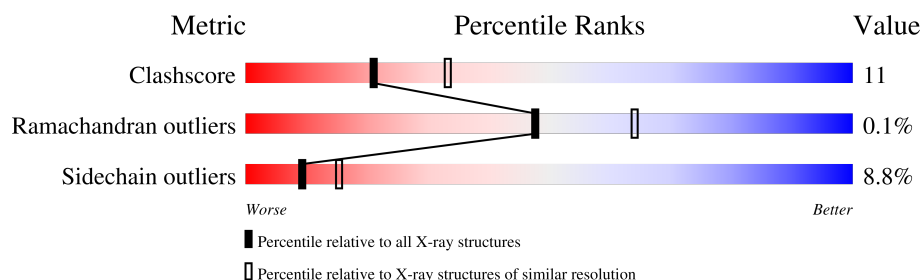
1 Overall quality at a glance

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	320	
1	B	320	
1	C	320	
1	D	320	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9371 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 6-PHOSPHOFRUCTOKINASE ISOZYME I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2255	1413	395	431	16			
1	B	301	Total	C	N	O	S	0	0	0
			2233	1401	390	426	16			
1	C	302	Total	C	N	O	S	0	0	1
			2251	1409	394	433	15			
1	D	305	Total	C	N	O	S	0	0	0
			2285	1432	396	441	16			

- Molecule 2 is water.

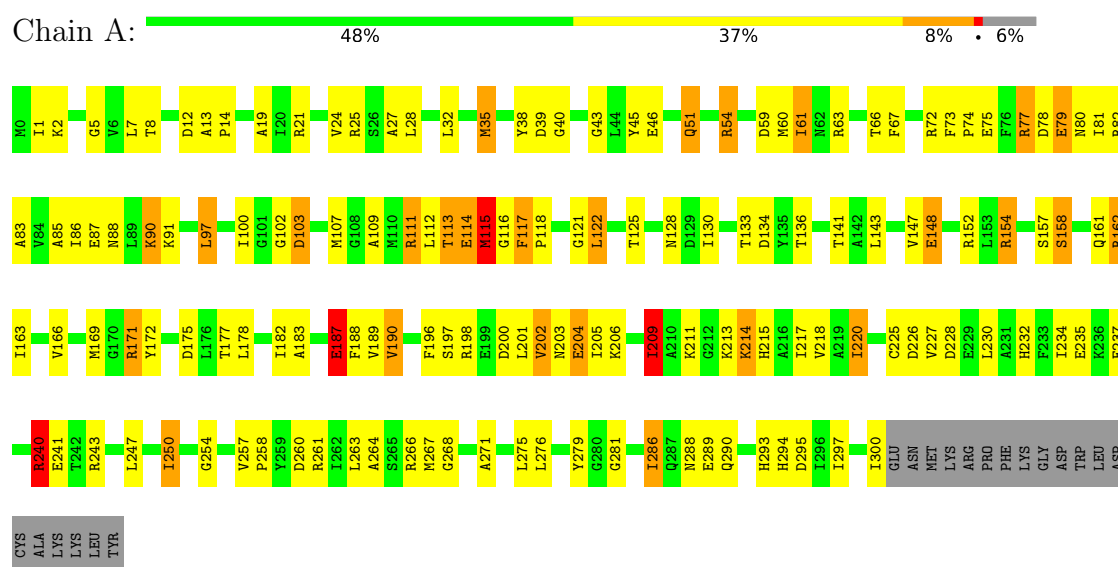
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	81	Total	O	0	0
			81	81		
2	B	76	Total	O	0	0
			76	76		
2	C	94	Total	O	0	0
			94	94		
2	D	96	Total	O	0	0
			96	96		

3 Residue-property plots

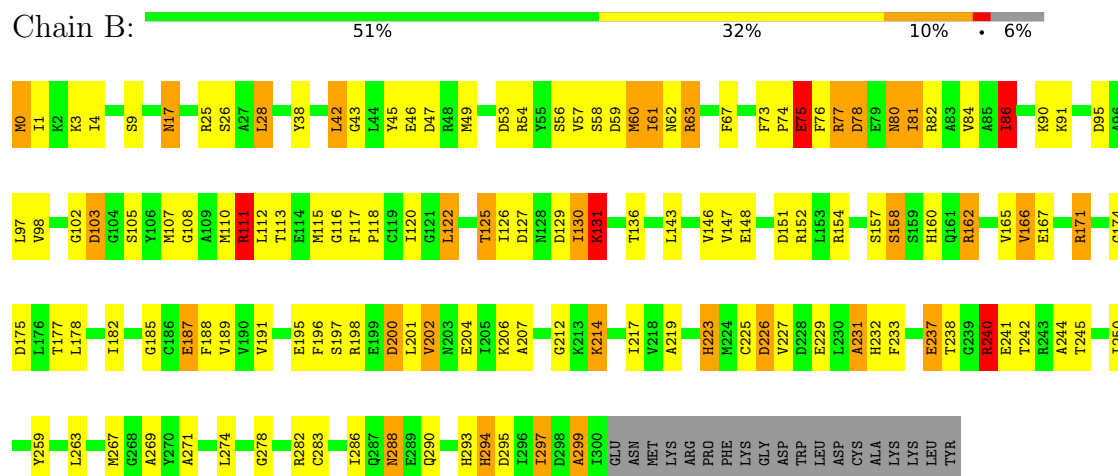
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: 6-PHOSPHOFRUCTOKINASE ISOZYME I

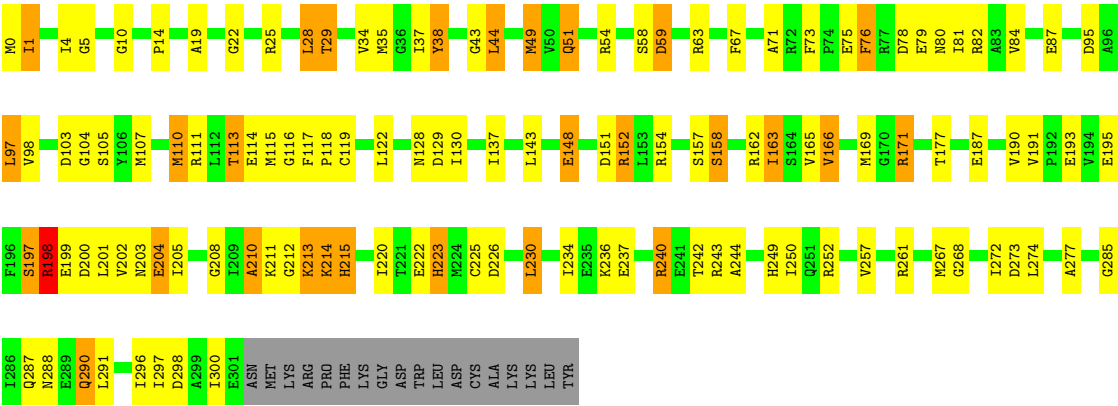


• Molecule 1: 6-PHOSPHOFRUCTOKINASE ISOZYME I

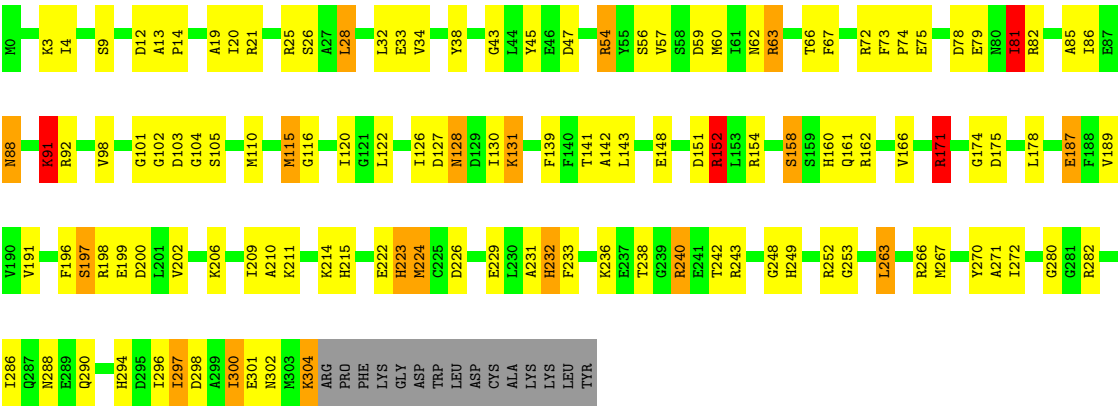


• Molecule 1: 6-PHOSPHOFRUCTOKINASE ISOZYME I





● Molecule 1: 6-PHOSPHOFRUCTOKINASE ISOZYME I



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	177.00Å 66.40Å 154.00Å 90.00° 118.80° 90.00°	Depositor
Resolution (Å)	100.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (100.00-2.40)	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	9371	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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	1.06	0/2286	2.37	123/3085 (4.0%)
1	B	1.04	0/2264	2.38	120/3057 (3.9%)
1	C	1.08	0/2282	2.36	129/3081 (4.2%)
1	D	1.05	1/2317 (0.0%)	2.31	126/3128 (4.0%)
All	All	1.05	1/9149 (0.0%)	2.35	498/12351 (4.0%)

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	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	73	PHE	CA-CB	-5.28	1.46	1.53

All (498) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ARG	CD-NE-CZ	22.09	155.32	124.40
1	B	152	ARG	CD-NE-CZ	19.73	152.02	124.40
1	A	103	ASP	CA-CB-CG	18.54	131.14	112.60
1	D	73	PHE	CA-CB-CG	13.51	127.31	113.80
1	D	187	GLU	CB-CG-CD	12.32	133.54	112.60
1	B	198	ARG	CA-C-N	12.23	137.07	120.44
1	B	198	ARG	C-N-CA	12.23	137.07	120.44
1	C	79	GLU	CA-CB-CG	11.32	136.75	114.10
1	D	243	ARG	CD-NE-CZ	11.31	140.24	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214	LYS	N-CA-C	11.11	123.08	110.97
1	B	78	ASP	CA-CB-CG	10.96	123.56	112.60
1	D	162	ARG	CD-NE-CZ	10.85	139.60	124.40
1	C	73	PHE	O-C-N	10.78	129.06	121.19
1	D	199	GLU	CB-CG-CD	10.49	130.43	112.60
1	C	211	LYS	CA-C-N	9.88	140.77	121.41
1	C	211	LYS	C-N-CA	9.88	140.77	121.41
1	D	199	GLU	CB-CA-C	9.72	126.15	110.88
1	A	152	ARG	NE-CZ-NH2	-9.63	110.53	119.20
1	D	91	LYS	CA-CB-CG	9.61	133.31	114.10
1	C	298	ASP	CA-CB-CG	9.57	122.17	112.60
1	B	80	ASN	CA-CB-CG	9.51	122.11	112.60
1	B	74	PRO	CA-C-N	9.26	133.89	120.38
1	B	74	PRO	C-N-CA	9.26	133.89	120.38
1	A	215	HIS	CA-C-O	9.07	131.66	121.51
1	D	243	ARG	NE-CZ-NH1	9.06	130.56	121.50
1	D	223	HIS	CA-CB-CG	-9.00	104.80	113.80
1	C	225	CYS	O-C-N	8.94	132.65	123.26
1	B	152	ARG	NE-CZ-NH2	-8.87	111.22	119.20
1	C	225	CYS	CB-CA-C	-8.85	93.83	111.17
1	A	51	GLN	CA-CB-CG	8.82	131.75	114.10
1	B	130	ILE	CA-C-O	8.82	130.04	120.43
1	A	198	ARG	CA-CB-CG	8.75	131.60	114.10
1	A	118	PRO	CA-C-O	8.73	130.99	121.03
1	C	187	GLU	CB-CG-CD	8.69	127.37	112.60
1	A	118	PRO	CB-CA-C	8.66	121.94	111.46
1	D	211	LYS	CA-C-N	8.63	134.89	120.91
1	D	211	LYS	C-N-CA	8.63	134.89	120.91
1	C	117	PHE	O-C-N	8.62	130.76	121.02
1	C	267	MET	CA-C-O	-8.52	111.92	120.70
1	C	80	ASN	CB-CA-C	8.37	127.49	109.99
1	B	212	GLY	N-CA-C	8.36	125.78	114.92
1	B	226	ASP	N-CA-C	-8.33	95.71	108.96
1	D	143	LEU	CA-C-O	-8.33	112.08	120.82
1	B	122	LEU	CB-CA-C	8.33	119.30	109.47
1	D	226	ASP	N-CA-C	-8.31	92.30	107.75
1	C	157	SER	CA-C-N	8.29	131.59	120.65
1	C	157	SER	C-N-CA	8.29	131.59	120.65
1	C	273	ASP	CA-CB-CG	8.24	120.84	112.60
1	B	59	ASP	N-CA-CB	-8.23	98.53	110.80
1	A	60	MET	N-CA-C	8.12	123.01	113.18
1	C	226	ASP	N-CA-C	-8.05	96.17	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	GLY	O-C-N	8.04	131.20	123.80
1	D	301	GLU	CA-C-N	8.03	131.69	120.29
1	D	301	GLU	C-N-CA	8.03	131.69	120.29
1	B	223	HIS	CA-CB-CG	-7.99	105.81	113.80
1	A	115	MET	CA-C-N	7.97	137.03	121.41
1	A	115	MET	C-N-CA	7.97	137.03	121.41
1	A	295	ASP	CA-CB-CG	-7.91	104.69	112.60
1	D	214	LYS	N-CA-C	7.88	119.95	111.36
1	B	167	GLU	CB-CG-CD	7.79	125.85	112.60
1	B	53	ASP	CA-CB-CG	7.77	120.37	112.60
1	B	151	ASP	CA-CB-CG	7.63	120.23	112.60
1	D	21	ARG	CA-C-N	7.62	128.38	120.00
1	D	21	ARG	C-N-CA	7.62	128.38	120.00
1	B	162	ARG	NE-CZ-NH1	-7.61	113.89	121.50
1	C	110	MET	N-CA-C	-7.58	102.62	111.03
1	D	60	MET	N-CA-C	7.57	122.81	112.90
1	C	1	ILE	N-CA-C	-7.56	96.95	107.99
1	B	58	SER	CA-C-N	7.52	134.03	122.29
1	B	58	SER	C-N-CA	7.52	134.03	122.29
1	B	157	SER	CA-C-N	7.46	130.50	120.65
1	B	157	SER	C-N-CA	7.46	130.50	120.65
1	A	2	LYS	CA-CB-CG	7.46	129.01	114.10
1	A	187	GLU	CB-CG-CD	7.45	125.26	112.60
1	A	175	ASP	O-C-N	7.42	130.02	122.08
1	A	148	GLU	N-CA-C	-7.40	103.30	111.36
1	D	12	ASP	CA-CB-CG	7.40	120.00	112.60
1	A	152	ARG	CG-CD-NE	-7.37	95.79	112.00
1	A	117	PHE	CA-CB-CG	-7.30	106.50	113.80
1	D	252	ARG	NE-CZ-NH2	7.29	125.76	119.20
1	B	195	GLU	N-CA-CB	7.25	120.62	109.97
1	D	63	ARG	NE-CZ-NH1	7.22	128.72	121.50
1	D	197	SER	N-CA-CB	7.19	123.25	110.80
1	C	210	ALA	N-CA-C	-7.19	103.38	111.07
1	B	86	ILE	CB-CA-C	7.18	122.14	112.22
1	A	220	ILE	CA-C-O	-7.17	112.87	120.76
1	D	210	ALA	CA-C-O	7.13	128.91	120.92
1	A	51	GLN	CB-CA-C	7.12	122.11	110.22
1	C	54	ARG	CD-NE-CZ	7.12	134.36	124.40
1	C	148	GLU	CB-CG-CD	7.10	124.67	112.60
1	A	158	SER	N-CA-CB	-7.10	99.28	110.28
1	C	193	GLU	CB-CG-CD	7.09	124.66	112.60
1	B	288	ASN	CA-C-N	7.06	134.13	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	ASN	C-N-CA	7.06	134.13	123.05
1	A	61	ILE	N-CA-C	7.04	119.85	111.05
1	B	237	GLU	N-CA-C	6.99	121.04	112.23
1	B	191	VAL	O-C-N	6.97	127.19	121.40
1	B	143	LEU	CA-C-N	6.94	130.15	120.29
1	B	143	LEU	C-N-CA	6.94	130.15	120.29
1	C	98	VAL	N-CA-CB	6.94	120.66	111.64
1	D	302	ASN	N-CA-C	6.91	118.89	111.36
1	C	111	ARG	CG-CD-NE	6.90	127.17	112.00
1	B	195	GLU	N-CA-C	-6.86	100.13	110.28
1	C	44	LEU	CA-C-N	6.83	129.99	120.29
1	C	44	LEU	C-N-CA	6.83	129.99	120.29
1	B	166	VAL	CB-CA-C	-6.81	100.55	110.63
1	C	215	HIS	CA-CB-CG	-6.81	106.99	113.80
1	B	187	GLU	CB-CG-CD	6.79	124.14	112.60
1	A	154	ARG	NE-CZ-NH2	-6.78	113.09	119.20
1	C	249	HIS	CA-CB-CG	-6.76	107.04	113.80
1	A	122	LEU	O-C-N	6.76	127.41	121.39
1	D	98	VAL	N-CA-CB	6.76	121.01	111.82
1	D	215	HIS	CA-CB-CG	-6.75	107.05	113.80
1	A	73	PHE	O-C-N	6.74	126.90	121.17
1	D	148	GLU	CB-CG-CD	6.72	124.03	112.60
1	C	98	VAL	O-C-N	6.72	130.33	123.20
1	A	54	ARG	CA-C-N	6.72	129.83	120.29
1	A	54	ARG	C-N-CA	6.72	129.83	120.29
1	C	237	GLU	N-CA-C	6.71	121.07	113.01
1	C	214	LYS	CA-C-O	6.70	128.04	121.00
1	C	130	ILE	O-C-N	6.68	130.72	123.03
1	D	304	LYS	CA-C-O	6.68	132.16	120.80
1	C	288	ASN	CA-CB-CG	-6.68	105.92	112.60
1	C	151	ASP	CA-CB-CG	6.67	119.27	112.60
1	D	79	GLU	CA-CB-CG	6.67	127.44	114.10
1	C	191	VAL	CA-C-N	6.66	126.60	119.28
1	C	191	VAL	C-N-CA	6.66	126.60	119.28
1	C	129	ASP	CA-CB-CG	-6.66	105.94	112.60
1	B	78	ASP	CA-C-N	6.65	129.49	120.38
1	B	78	ASP	C-N-CA	6.65	129.49	120.38
1	B	225	CYS	O-C-N	6.65	130.24	123.26
1	B	26	SER	O-C-N	6.64	129.26	122.09
1	A	237	GLU	N-CA-C	6.63	121.11	112.89
1	D	229	GLU	N-CA-C	-6.62	103.98	111.14
1	A	268	GLY	O-C-N	6.61	128.54	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ASP	N-CA-CB	6.59	119.76	109.94
1	D	290	GLN	CB-CG-CD	-6.58	101.42	112.60
1	C	0	MET	CA-C-N	6.56	131.30	122.90
1	C	0	MET	C-N-CA	6.56	131.30	122.90
1	D	142	ALA	O-C-N	6.53	128.79	122.07
1	A	97	LEU	N-CA-CB	-6.52	99.46	111.13
1	B	217	ILE	CA-C-N	6.51	131.97	123.11
1	B	217	ILE	C-N-CA	6.51	131.97	123.11
1	A	79	GLU	CA-CB-CG	6.50	127.10	114.10
1	A	152	ARG	NE-CZ-NH1	6.46	127.96	121.50
1	A	67	PHE	CA-CB-CG	6.44	120.24	113.80
1	C	76	PHE	CA-CB-CG	6.43	120.23	113.80
1	B	175	ASP	O-C-N	6.42	128.95	122.08
1	A	162	ARG	CD-NE-CZ	6.41	133.37	124.40
1	B	78	ASP	CB-CA-C	6.41	119.38	110.16
1	B	191	VAL	N-CA-CB	-6.40	107.41	111.83
1	B	295	ASP	N-CA-C	-6.40	100.81	110.28
1	D	62	ASN	OD1-CG-ND2	-6.37	116.23	122.60
1	C	287	GLN	N-CA-CB	6.36	120.75	110.77
1	D	154	ARG	CA-C-N	6.34	128.69	120.44
1	D	154	ARG	C-N-CA	6.34	128.69	120.44
1	C	223	HIS	CA-CB-CG	-6.34	107.46	113.80
1	C	137	ILE	N-CA-CB	6.33	118.10	110.31
1	A	78	ASP	CA-C-O	6.33	127.52	120.43
1	B	196	PHE	CA-C-N	-6.32	114.09	123.00
1	B	196	PHE	C-N-CA	-6.32	114.09	123.00
1	A	232	HIS	N-CA-CB	6.32	119.17	110.01
1	B	3	LYS	CB-CA-C	-6.32	100.03	110.14
1	A	226	ASP	N-CA-C	-6.31	96.02	107.75
1	D	25	ARG	CA-C-O	-6.30	113.87	120.55
1	C	58	SER	CA-C-O	-6.26	113.86	120.63
1	B	67	PHE	CA-CB-CG	6.24	120.04	113.80
1	A	211	LYS	CA-C-N	6.24	130.61	122.26
1	A	211	LYS	C-N-CA	6.24	130.61	122.26
1	A	227	VAL	CA-C-O	-6.23	113.91	120.57
1	B	147	VAL	O-C-N	-6.22	115.84	121.87
1	C	213	LYS	CA-CB-CG	6.22	126.53	114.10
1	A	213	LYS	N-CA-C	-6.21	99.88	109.76
1	B	130	ILE	CA-C-N	6.21	130.30	121.42
1	B	130	ILE	C-N-CA	6.21	130.30	121.42
1	A	225	CYS	O-C-N	6.21	130.24	123.10
1	C	71	ALA	CA-C-O	6.20	127.94	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	GLU	CA-C-N	6.20	132.54	122.81
1	A	187	GLU	C-N-CA	6.20	132.54	122.81
1	D	226	ASP	CA-C-O	-6.19	114.15	120.84
1	B	177	THR	CA-C-O	6.19	127.11	120.55
1	C	230	LEU	CA-C-N	6.18	128.48	120.44
1	C	230	LEU	C-N-CA	6.18	128.48	120.44
1	C	169	MET	CA-C-O	6.18	128.86	121.88
1	C	38	TYR	CA-C-N	6.18	130.90	122.07
1	C	38	TYR	C-N-CA	6.18	130.90	122.07
1	B	127	ASP	N-CA-C	6.18	120.65	113.18
1	A	227	VAL	O-C-N	6.16	128.09	121.87
1	B	103	ASP	N-CA-C	-6.15	104.57	111.28
1	A	78	ASP	CA-C-N	6.15	128.81	120.38
1	A	78	ASP	C-N-CA	6.15	128.81	120.38
1	B	288	ASN	CA-CB-CG	-6.15	106.45	112.60
1	D	214	LYS	CA-C-O	6.13	126.92	120.42
1	B	299	ALA	N-CA-C	-6.11	104.89	112.90
1	C	59	ASP	CA-CB-CG	6.10	118.70	112.60
1	C	152	ARG	CA-C-N	6.09	128.93	120.29
1	C	152	ARG	C-N-CA	6.09	128.93	120.29
1	A	51	GLN	CB-CG-CD	6.08	122.94	112.60
1	A	190	VAL	CA-C-O	6.08	126.27	120.31
1	A	158	SER	CB-CA-C	6.08	122.34	110.67
1	C	80	ASN	N-CA-C	-6.07	105.37	112.89
1	B	259	TYR	CA-C-N	6.06	128.40	120.28
1	B	259	TYR	C-N-CA	6.06	128.40	120.28
1	B	174	GLY	CA-C-N	6.05	129.20	120.79
1	B	174	GLY	C-N-CA	6.05	129.20	120.79
1	B	152	ARG	NE-CZ-NH1	6.04	127.54	121.50
1	C	25	ARG	CA-C-N	6.03	128.64	120.44
1	C	25	ARG	C-N-CA	6.03	128.64	120.44
1	D	98	VAL	N-CA-C	-6.03	98.84	107.77
1	A	196	PHE	CA-CB-CG	6.03	119.83	113.80
1	B	182	ILE	O-C-N	6.02	128.16	121.90
1	B	202	VAL	CB-CA-C	6.02	120.53	112.22
1	B	62	ASN	CA-C-N	6.02	131.00	122.09
1	B	62	ASN	C-N-CA	6.02	131.00	122.09
1	C	163	ILE	N-CA-CB	6.01	118.21	110.99
1	B	160	HIS	N-CA-C	6.01	121.35	113.30
1	A	97	LEU	N-CA-C	6.00	119.26	109.06
1	B	226	ASP	N-CA-CB	6.00	120.25	110.17
1	B	131	LYS	CG-CD-CE	6.00	125.10	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	MET	O-C-N	6.00	128.57	122.09
1	D	148	GLU	CB-CA-C	6.00	120.74	110.79
1	A	243	ARG	NE-CZ-NH1	5.99	127.49	121.50
1	D	158	SER	CB-CA-C	-5.98	101.48	110.88
1	D	199	GLU	CG-CD-OE1	5.97	132.14	118.40
1	D	175	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	232	HIS	CA-C-O	-5.97	114.55	120.82
1	D	162	ARG	CB-CA-C	-5.97	98.08	109.66
1	A	21	ARG	CA-C-N	5.96	126.56	119.94
1	A	21	ARG	C-N-CA	5.96	126.56	119.94
1	C	195	GLU	CB-CG-CD	5.96	122.73	112.60
1	C	143	LEU	CA-C-N	5.96	128.54	120.44
1	C	143	LEU	C-N-CA	5.96	128.54	120.44
1	D	189	VAL	CA-C-N	5.96	131.33	123.11
1	D	189	VAL	C-N-CA	5.96	131.33	123.11
1	D	120	ILE	N-CA-CB	5.96	120.21	111.52
1	A	46	GLU	CB-CG-CD	5.95	122.72	112.60
1	A	189	VAL	CA-C-N	5.95	131.32	123.11
1	A	189	VAL	C-N-CA	5.95	131.32	123.11
1	A	260	ASP	N-CA-CB	5.94	118.95	110.16
1	C	177	THR	CA-CB-OG1	-5.94	100.69	109.60
1	D	127	ASP	N-CA-C	5.93	120.38	113.20
1	B	200	ASP	N-CA-CB	5.92	119.46	110.28
1	D	148	GLU	O-C-N	-5.92	115.84	122.12
1	A	293	HIS	CA-C-N	5.92	131.88	122.59
1	A	293	HIS	C-N-CA	5.92	131.88	122.59
1	D	152	ARG	NE-CZ-NH2	-5.92	113.87	119.20
1	D	166	VAL	CA-C-O	-5.92	114.24	120.39
1	B	17	ASN	CA-C-O	-5.91	114.15	120.42
1	A	254	GLY	N-CA-C	5.91	118.07	112.04
1	D	301	GLU	N-CA-C	5.91	120.60	111.56
1	B	136	THR	CA-CB-OG1	-5.90	100.75	109.60
1	D	85	ALA	CA-C-N	5.90	128.55	120.46
1	D	85	ALA	C-N-CA	5.90	128.55	120.46
1	C	104	GLY	N-CA-C	-5.89	105.67	112.50
1	C	187	GLU	CG-CD-OE1	5.89	131.95	118.40
1	D	59	ASP	CA-CB-CG	5.89	118.49	112.60
1	D	152	ARG	CG-CD-NE	-5.88	99.06	112.00
1	B	25	ARG	CA-C-N	5.86	128.41	120.44
1	B	25	ARG	C-N-CA	5.86	128.41	120.44
1	C	98	VAL	CA-C-O	-5.86	114.29	120.39
1	C	290	GLN	N-CA-CB	5.84	120.09	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ARG	CD-NE-CZ	5.82	132.54	124.40
1	A	250	ILE	CA-C-N	5.81	128.65	120.28
1	A	250	ILE	C-N-CA	5.81	128.65	120.28
1	D	229	GLU	CB-CA-C	5.80	120.07	110.90
1	B	269	ALA	CA-C-N	5.80	128.05	120.28
1	B	269	ALA	C-N-CA	5.80	128.05	120.28
1	D	128	ASN	CA-C-N	5.79	132.61	121.54
1	D	128	ASN	C-N-CA	5.79	132.61	121.54
1	D	224	MET	N-CA-C	-5.79	105.23	112.93
1	D	288	ASN	OD1-CG-ND2	5.78	128.38	122.60
1	D	126	ILE	CA-C-O	-5.78	114.23	120.47
1	D	174	GLY	CA-C-N	5.76	130.35	121.19
1	D	174	GLY	C-N-CA	5.76	130.35	121.19
1	C	277	ALA	CA-C-O	5.76	126.30	119.56
1	D	166	VAL	O-C-N	5.75	129.29	123.20
1	D	253	GLY	N-CA-C	5.75	121.57	111.57
1	A	215	HIS	CA-CB-CG	-5.74	108.06	113.80
1	B	171	ARG	N-CA-C	5.73	117.99	111.11
1	D	54	ARG	CB-CA-C	-5.73	99.34	110.46
1	C	222	GLU	CG-CD-OE2	-5.73	105.22	118.40
1	C	116	GLY	N-CA-C	5.73	124.00	115.64
1	D	242	THR	CA-CB-OG1	-5.72	101.02	109.60
1	D	74	PRO	CA-C-O	5.72	127.01	119.00
1	A	182	ILE	N-CA-C	5.72	115.90	110.53
1	A	88	ASN	O-C-N	5.70	127.94	122.07
1	B	283	CYS	CB-CA-C	5.69	120.93	109.38
1	D	151	ASP	CA-CB-CG	5.68	118.28	112.60
1	D	280	GLY	CA-C-O	-5.67	115.19	121.37
1	D	74	PRO	CB-CA-C	5.67	119.96	111.68
1	C	250	ILE	CA-C-N	5.66	128.43	120.28
1	C	250	ILE	C-N-CA	5.66	128.43	120.28
1	B	73	PHE	O-C-N	5.66	125.53	121.12
1	A	294	HIS	CA-CB-CG	-5.66	108.14	113.80
1	C	14	PRO	CA-C-O	-5.65	115.18	121.23
1	D	210	ALA	CA-C-N	5.65	134.75	121.52
1	D	210	ALA	C-N-CA	5.65	134.75	121.52
1	D	158	SER	N-CA-C	5.65	117.12	111.07
1	A	177	THR	N-CA-C	5.64	117.88	111.11
1	C	34	VAL	CA-C-O	5.63	126.32	120.36
1	D	270	TYR	CA-C-N	5.62	127.81	120.28
1	D	270	TYR	C-N-CA	5.62	127.81	120.28
1	A	133	THR	CA-CB-OG1	-5.62	101.17	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	GLU	CA-C-N	5.62	129.59	120.60
1	B	75	GLU	C-N-CA	5.62	129.59	120.60
1	D	88	ASN	CA-C-O	-5.61	114.60	120.55
1	B	295	ASP	CB-CA-C	5.61	119.25	109.65
1	B	245	THR	O-C-N	5.61	129.88	123.31
1	C	113	THR	CA-C-N	5.61	127.79	120.28
1	C	113	THR	C-N-CA	5.61	127.79	120.28
1	D	196	PHE	N-CA-C	5.57	117.98	108.90
1	D	297	ILE	O-C-N	5.56	127.36	121.91
1	D	187	GLU	CA-CB-CG	5.56	125.22	114.10
1	D	248	GLY	CA-C-N	5.55	129.57	120.63
1	D	248	GLY	C-N-CA	5.55	129.57	120.63
1	A	35	MET	N-CA-CB	5.55	119.31	110.65
1	B	129	ASP	CA-C-N	5.55	130.80	122.75
1	B	129	ASP	C-N-CA	5.55	130.80	122.75
1	C	151	ASP	CA-C-N	5.55	127.71	120.28
1	C	151	ASP	C-N-CA	5.55	127.71	120.28
1	B	278	GLY	CA-C-O	-5.54	112.87	119.07
1	C	107	MET	CA-C-O	5.53	126.29	120.42
1	C	28	LEU	CA-C-N	5.53	127.69	120.28
1	C	28	LEU	C-N-CA	5.53	127.69	120.28
1	A	152	ARG	N-CA-CB	5.53	118.34	110.16
1	B	294	HIS	CB-CA-C	-5.52	98.47	109.79
1	B	120	ILE	N-CA-CB	5.52	119.58	111.52
1	D	191	VAL	N-CA-CB	-5.51	108.02	111.83
1	B	116	GLY	N-CA-C	5.51	124.04	115.72
1	A	79	GLU	CB-CG-CD	5.51	121.97	112.60
1	B	152	ARG	CG-CD-NE	-5.51	99.88	112.00
1	C	198	ARG	CA-C-N	5.51	128.11	120.29
1	C	198	ARG	C-N-CA	5.51	128.11	120.29
1	D	198	ARG	CA-C-O	5.50	126.57	120.63
1	D	171	ARG	NE-CZ-NH1	5.50	127.00	121.50
1	C	10	GLY	CA-C-N	-5.49	114.71	120.31
1	C	10	GLY	C-N-CA	-5.49	114.71	120.31
1	D	171	ARG	CD-NE-CZ	5.49	132.08	124.40
1	D	296	ILE	N-CA-C	5.48	116.21	110.62
1	B	166	VAL	O-C-N	5.48	129.18	123.26
1	C	148	GLU	CA-C-N	5.48	128.07	120.29
1	C	148	GLU	C-N-CA	5.48	128.07	120.29
1	D	81	ILE	CB-CA-C	5.47	119.58	112.24
1	A	203	ASN	CA-C-N	5.47	127.61	120.28
1	A	203	ASN	C-N-CA	5.47	127.61	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	263	LEU	O-C-N	5.46	127.70	122.07
1	A	112	LEU	N-CA-C	-5.46	106.12	112.89
1	A	206	LYS	CA-C-N	5.45	127.53	120.44
1	A	206	LYS	C-N-CA	5.45	127.53	120.44
1	D	232	HIS	N-CA-CB	5.45	118.13	110.12
1	A	209	ILE	O-C-N	5.45	127.84	121.96
1	C	67	PHE	CA-CB-CG	5.44	119.24	113.80
1	D	116	GLY	N-CA-C	5.44	123.46	115.08
1	D	231	ALA	CA-C-N	5.43	127.56	120.28
1	D	231	ALA	C-N-CA	5.43	127.56	120.28
1	D	20	ILE	N-CA-CB	5.42	116.53	110.62
1	B	47	ASP	N-CA-C	5.42	118.91	111.54
1	A	88	ASN	OD1-CG-ND2	5.42	128.02	122.60
1	D	19	ALA	N-CA-C	-5.42	105.29	111.14
1	D	88	ASN	O-C-N	5.42	127.86	122.12
1	D	160	HIS	CA-C-O	-5.41	112.98	119.15
1	C	105	SER	CA-C-N	5.41	129.75	120.72
1	C	105	SER	C-N-CA	5.41	129.75	120.72
1	D	104	GLY	N-CA-C	-5.41	106.24	112.83
1	B	111	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	A	178	LEU	CB-CA-C	5.40	120.03	110.85
1	C	187	GLU	OE1-CD-OE2	-5.40	109.94	122.90
1	C	54	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	C	103	ASP	CB-CA-C	5.39	121.25	109.99
1	A	24	VAL	N-CA-C	5.38	115.59	110.42
1	B	3	LYS	N-CA-C	5.38	117.17	108.34
1	B	125	THR	CA-CB-CG2	5.38	119.65	110.50
1	B	185	GLY	N-CA-C	-5.38	106.79	115.08
1	C	204	GLU	CB-CA-C	-5.38	101.86	110.79
1	B	178	LEU	N-CA-CB	-5.36	102.23	110.01
1	A	113	THR	N-CA-C	-5.36	105.35	111.14
1	C	291	LEU	CA-C-O	5.36	126.97	120.81
1	C	296	ILE	CA-C-O	-5.36	115.48	121.05
1	A	157	SER	CA-C-O	5.35	126.22	120.70
1	B	162	ARG	CD-NE-CZ	-5.35	116.91	124.40
1	D	141	THR	CA-CB-OG1	-5.34	101.59	109.60
1	A	198	ARG	CB-CA-C	-5.34	102.27	110.81
1	B	75	GLU	CA-CB-CG	5.34	124.78	114.10
1	C	54	ARG	CA-CB-CG	5.34	124.78	114.10
1	C	59	ASP	CB-CA-C	5.33	121.03	110.42
1	A	171	ARG	O-C-N	5.33	128.24	122.11
1	C	37	ILE	CA-C-N	5.33	130.24	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	ILE	C-N-CA	5.33	130.24	121.39
1	D	131	LYS	CA-CB-CG	5.33	124.76	114.10
1	C	54	ARG	CB-CA-C	-5.32	101.63	110.68
1	B	126	ILE	CA-C-O	-5.32	114.50	120.25
1	B	80	ASN	CA-C-N	5.31	127.73	120.46
1	B	80	ASN	C-N-CA	5.31	127.73	120.46
1	D	141	THR	CA-C-N	5.31	127.34	120.44
1	D	141	THR	C-N-CA	5.31	127.34	120.44
1	A	113	THR	CB-CA-C	5.30	119.28	110.90
1	D	67	PHE	N-CA-CB	5.30	118.50	110.28
1	A	51	GLN	CA-C-N	5.30	130.03	122.72
1	A	51	GLN	C-N-CA	5.30	130.03	122.72
1	D	152	ARG	CA-C-N	5.29	127.37	120.28
1	D	152	ARG	C-N-CA	5.29	127.37	120.28
1	D	25	ARG	NH1-CZ-NH2	5.28	126.16	119.30
1	D	34	VAL	N-CA-C	5.28	115.50	108.11
1	C	128	ASN	N-CA-CB	-5.27	104.72	112.78
1	A	202	VAL	CB-CA-C	5.26	119.24	112.14
1	A	72	ARG	N-CA-CB	5.25	118.94	110.65
1	B	274	LEU	O-C-N	5.25	128.13	122.15
1	C	73	PHE	CA-CB-CG	5.24	119.04	113.80
1	C	171	ARG	CD-NE-CZ	-5.24	117.06	124.40
1	D	266	ARG	CB-CG-CD	5.24	123.36	111.30
1	D	296	ILE	CA-C-N	5.24	127.16	120.56
1	D	296	ILE	C-N-CA	5.24	127.16	120.56
1	B	162	ARG	NH1-CZ-NH2	5.24	126.11	119.30
1	C	285	GLY	CA-C-N	5.23	130.33	123.11
1	C	285	GLY	C-N-CA	5.23	130.33	123.11
1	D	25	ARG	NE-CZ-NH2	-5.23	114.50	119.20
1	B	146	VAL	CA-C-O	-5.22	115.63	121.17
1	D	33	GLU	CA-C-N	-5.22	116.31	123.14
1	D	33	GLU	C-N-CA	-5.22	116.31	123.14
1	A	232	HIS	O-C-N	5.21	127.44	122.07
1	C	103	ASP	CA-C-N	5.21	125.73	119.94
1	C	103	ASP	C-N-CA	5.21	125.73	119.94
1	C	152	ARG	CD-NE-CZ	-5.21	117.11	124.40
1	A	235	GLU	CA-C-O	-5.20	114.91	120.42
1	A	134	ASP	N-CA-C	-5.20	105.50	111.07
1	B	57	VAL	CA-C-N	5.20	129.00	120.63
1	B	57	VAL	C-N-CA	5.20	129.00	120.63
1	B	63	ARG	N-CA-CB	-5.20	101.81	110.23
1	D	224	MET	CA-CB-CG	-5.20	103.70	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	210	ALA	CA-C-O	-5.19	115.37	120.82
1	D	57	VAL	CA-C-N	5.19	127.95	120.38
1	D	57	VAL	C-N-CA	5.19	127.95	120.38
1	D	63	ARG	N-CA-CB	-5.18	101.97	110.52
1	A	39	ASP	N-CA-C	5.18	118.53	111.39
1	B	60	MET	N-CA-C	5.18	119.31	112.89
1	B	231	ALA	CB-CA-C	5.17	119.38	110.79
1	D	249	HIS	CA-CB-CG	-5.17	108.63	113.80
1	A	198	ARG	CA-C-N	5.16	127.97	120.79
1	A	198	ARG	C-N-CA	5.16	127.97	120.79
1	A	12	ASP	CB-CA-C	5.16	120.33	109.65
1	C	197	SER	N-CA-CB	5.16	118.70	110.65
1	C	272	ILE	CA-C-N	5.15	127.19	120.28
1	C	272	ILE	C-N-CA	5.15	127.19	120.28
1	C	199	GLU	CB-CG-CD	5.15	121.36	112.60
1	A	87	GLU	CA-C-N	5.15	127.13	120.44
1	A	87	GLU	C-N-CA	5.15	127.13	120.44
1	D	162	ARG	CG-CD-NE	-5.15	100.68	112.00
1	A	213	LYS	N-CA-CB	5.14	117.92	109.95
1	C	4	ILE	O-C-N	5.12	128.41	123.03
1	B	293	HIS	CA-CB-CG	-5.12	108.68	113.80
1	B	250	ILE	CA-C-N	5.11	127.13	120.28
1	B	250	ILE	C-N-CA	5.11	127.13	120.28
1	A	25	ARG	CA-C-N	5.11	127.39	120.44
1	A	25	ARG	C-N-CA	5.11	127.39	120.44
1	D	199	GLU	CA-C-O	-5.11	115.46	120.82
1	A	209	ILE	N-CA-CB	5.11	115.98	110.62
1	C	84	VAL	CA-C-N	5.10	127.08	120.44
1	C	84	VAL	C-N-CA	5.10	127.08	120.44
1	B	240	ARG	CG-CD-NE	5.10	123.23	112.00
1	C	14	PRO	CB-CA-C	5.10	118.07	111.64
1	C	243	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	B	77	ARG	N-CA-C	-5.10	105.63	111.14
1	C	203	ASN	CA-C-N	5.10	127.11	120.28
1	C	203	ASN	C-N-CA	5.10	127.11	120.28
1	C	211	LYS	CA-CB-CG	5.09	124.29	114.10
1	A	228	ASP	CB-CA-C	5.09	118.88	110.88
1	A	109	ALA	N-CA-C	-5.09	105.43	111.69
1	B	98	VAL	N-CA-CB	5.09	118.08	111.67
1	A	240	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	C	19	ALA	N-CA-C	-5.08	105.65	111.14
1	D	20	ILE	CA-C-O	-5.08	115.86	121.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	HIS	N-CA-CB	5.07	117.53	109.82
1	A	46	GLU	CG-CD-OE2	-5.07	106.74	118.40
1	B	290	GLN	CB-CA-C	5.07	119.06	109.37
1	A	114	GLU	O-C-N	-5.07	115.85	122.59
1	A	97	LEU	O-C-N	5.06	129.45	123.33
1	C	274	LEU	CA-C-N	5.05	127.01	120.44
1	C	274	LEU	C-N-CA	5.05	127.01	120.44
1	A	148	GLU	CA-C-O	-5.05	115.07	120.42
1	A	90	LYS	N-CA-CB	5.05	117.28	109.91
1	C	166	VAL	N-CA-C	5.04	115.11	107.80
1	A	77	ARG	N-CA-C	-5.04	106.39	112.54
1	A	115	MET	O-C-N	-5.03	115.89	122.59
1	B	238	THR	CA-CB-OG1	-5.03	102.06	109.60
1	D	45	TYR	CA-C-N	5.03	132.36	122.31
1	D	45	TYR	C-N-CA	5.03	132.36	122.31
1	A	13	ALA	O-C-N	5.02	127.18	122.06
1	C	22	GLY	CA-C-N	5.02	126.89	120.56
1	C	22	GLY	C-N-CA	5.02	126.89	120.56
1	A	220	ILE	O-C-N	5.02	128.62	123.05
1	B	178	LEU	CB-CA-C	5.02	118.76	110.88
1	B	136	THR	CA-C-N	5.01	128.70	121.18
1	B	136	THR	C-N-CA	5.01	128.70	121.18
1	D	72	ARG	CA-C-O	-5.01	115.21	120.58
1	A	12	ASP	CA-C-O	5.01	127.38	121.87
1	C	29	THR	CA-CB-CG2	5.00	119.01	110.50
1	A	79	GLU	CA-C-N	5.00	127.48	120.28
1	A	79	GLU	C-N-CA	5.00	127.48	120.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	300	ILE	Mainchain
1	D	152	ARG	Sidechain

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	2255	0	2250	63	1
1	B	2233	0	2212	67	0
1	C	2251	0	2240	39	2
1	D	2285	0	2262	36	1
2	A	81	0	0	2	0
2	B	76	0	0	4	0
2	C	94	0	0	5	0
2	D	96	0	0	2	1
All	All	9371	0	8964	198	3

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 11.

All (198) 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:131:LYS:H	1:B:131:LYS:HD2	1.09	1.09
1:A:240:ARG:HG2	1:A:240:ARG:HH11	1.17	1.08
1:C:240:ARG:HH11	1:C:240:ARG:HG2	1.28	0.95
1:B:75:GLU:HB3	1:B:81:ILE:HD13	1.58	0.84
1:B:131:LYS:HD2	1:B:131:LYS:N	1.93	0.81
1:C:190:VAL:HB	1:C:220:ILE:HG13	1.64	0.77
1:C:240:ARG:HG2	1:C:240:ARG:NH1	1.98	0.76
1:B:110:MET:HG2	1:B:297:ILE:HD11	1.68	0.75
1:B:240:ARG:HH11	1:B:240:ARG:HG2	1.51	0.74
1:C:240:ARG:HH11	1:C:240:ARG:CG	2.01	0.74
1:A:240:ARG:HG2	1:A:240:ARG:NH1	1.95	0.73
1:D:88:ASN:HA	1:D:91:LYS:HG3	1.70	0.73
1:A:111:ARG:HG3	1:A:111:ARG:HH11	1.54	0.72
1:B:110:MET:HG2	1:B:297:ILE:CD1	2.20	0.72
1:B:38:TYR:O	1:B:43:GLY:HA3	1.91	0.71
1:C:115:MET:HE3	2:C:413:HOH:O	1.90	0.70
1:B:197:SER:HB3	1:B:200:ASP:OD2	1.91	0.70
1:B:162:ARG:NH1	2:B:383:HOH:O	2.20	0.69
1:D:240:ARG:HG2	1:D:240:ARG:HH11	1.57	0.69
1:B:263:LEU:HD11	1:B:267:MET:HE3	1.75	0.68
1:C:208:GLY:O	1:C:213:LYS:HB3	1.95	0.68
1:B:0:MET:HA	1:B:0:MET:HE2	1.77	0.67
1:A:114:GLU:O	1:A:116:GLY:N	2.29	0.66
1:B:154:ARG:O	1:B:158:SER:HB2	1.96	0.66
1:B:82:ARG:HH21	1:B:115:MET:HE1	1.61	0.65
1:B:131:LYS:H	1:B:131:LYS:CD	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ILE:HG12	1:B:117:PHE:CE1	2.32	0.64
1:D:197:SER:HB3	1:D:200:ASP:OD2	1.97	0.64
1:D:200:ASP:HB3	2:D:407:HOH:O	1.99	0.63
1:B:111:ARG:O	1:B:115:MET:HG3	1.99	0.62
1:C:162:ARG:NH1	2:C:394:HOH:O	2.20	0.62
1:B:200:ASP:O	1:B:204:GLU:HG2	1.99	0.62
1:B:86:ILE:HG12	1:B:117:PHE:HE1	1.62	0.62
1:C:38:TYR:O	1:C:43:GLY:HA3	1.99	0.61
1:B:76:PHE:HZ	1:B:112:LEU:HD11	1.64	0.61
1:A:214:LYS:HA	1:A:240:ARG:HH22	1.66	0.60
1:A:86:ILE:HD11	1:A:115:MET:SD	2.41	0.60
1:B:131:LYS:HD3	1:B:299:ALA:O	2.02	0.60
1:D:115:MET:HA	1:D:115:MET:CE	2.33	0.59
1:D:240:ARG:HG2	1:D:240:ARG:NH1	2.16	0.59
1:B:78:ASP:OD1	1:B:80:ASN:HB3	2.02	0.59
1:D:82:ARG:O	1:D:86:ILE:HG13	2.03	0.59
1:B:102:GLY:HA2	1:B:130:ILE:HD11	1.83	0.59
1:B:202:VAL:HG21	1:B:233:PHE:CE2	2.38	0.59
1:D:26:SER:HB2	1:D:272:ILE:HG13	1.84	0.58
1:D:75:GLU:O	1:D:81:ILE:HG21	2.03	0.58
1:A:82:ARG:HE	1:A:115:MET:CE	2.17	0.58
1:B:125:THR:HG22	1:B:130:ILE:HD12	1.85	0.57
1:C:190:VAL:CB	1:C:220:ILE:HG13	2.32	0.57
1:A:288:ASN:HB3	1:B:288:ASN:ND2	2.20	0.57
1:B:82:ARG:HH21	1:B:115:MET:CE	2.18	0.57
1:D:115:MET:HA	1:D:115:MET:HE2	1.87	0.57
1:A:163:ILE:HD12	1:A:240:ARG:HB3	1.87	0.56
1:A:38:TYR:O	1:A:43:GLY:HA3	2.05	0.56
1:D:9:SER:HB3	1:D:105:SER:HB2	1.87	0.56
1:A:171:ARG:HD3	1:A:172:TYR:CZ	2.41	0.56
1:A:154:ARG:O	1:A:158:SER:HB3	2.05	0.56
1:A:122:LEU:HD21	1:A:271:ALA:HB2	1.87	0.55
1:D:38:TYR:O	1:D:43:GLY:HA3	2.06	0.55
1:D:202:VAL:HG21	1:D:233:PHE:CE2	2.43	0.54
1:C:214:LYS:O	1:C:240:ARG:NH1	2.40	0.53
1:A:161:GLN:HG2	1:A:214:LYS:HB2	1.90	0.53
1:B:9:SER:HB3	1:B:105:SER:HB3	1.90	0.53
1:B:226:ASP:HB3	1:B:229:GLU:HB2	1.89	0.53
1:A:214:LYS:O	1:A:240:ARG:NH1	2.42	0.52
1:D:282:ARG:HA	1:D:294:HIS:O	2.09	0.52
1:A:286:ILE:HD11	1:A:289:GLU:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ASN:HB3	1:B:288:ASN:HB3	1.93	0.51
1:C:35:MET:HE3	1:C:49:MET:HB2	1.93	0.51
1:A:28:LEU:HD23	1:A:54:ARG:HG2	1.92	0.51
1:C:201:LEU:O	1:C:205:ILE:HG13	2.10	0.51
1:A:230:LEU:O	1:A:234:ILE:HG13	2.11	0.51
1:B:108:GLY:O	1:B:112:LEU:HD12	2.11	0.51
1:A:188:PHE:HB2	1:A:218:VAL:HG22	1.93	0.50
1:A:51:GLN:NE2	2:A:327:HOH:O	2.44	0.50
1:C:154:ARG:HH11	1:C:215:HIS:CD2	2.29	0.50
1:A:169:MET:HE2	2:A:383:HOH:O	2.11	0.50
1:B:188:PHE:CE1	1:B:204:GLU:HB3	2.46	0.50
1:D:78:ASP:O	1:D:81:ILE:HG22	2.11	0.50
1:C:76:PHE:O	1:C:82:ARG:HD3	2.11	0.50
1:D:263:LEU:HD11	1:D:267:MET:HE3	1.94	0.50
1:B:204:GLU:O	1:B:207:ALA:HB3	2.11	0.49
1:C:190:VAL:CG1	1:C:220:ILE:HG13	2.42	0.49
1:D:9:SER:O	1:D:101:GLY:HA3	2.13	0.49
1:B:162:ARG:NE	1:B:241:GLU:OE2	2.46	0.49
1:A:45:TYR:CD1	1:A:81:ILE:HG23	2.48	0.49
1:B:282:ARG:HA	1:B:294:HIS:O	2.13	0.49
1:B:28:LEU:HD23	1:B:54:ARG:HG3	1.95	0.49
1:D:171:ARG:HG2	1:D:223:HIS:CD2	2.48	0.49
1:A:263:LEU:HD11	1:A:267:MET:HE3	1.94	0.49
1:A:257:VAL:O	1:A:261:ARG:HG3	2.13	0.48
1:D:128:ASN:HB2	1:D:139:PHE:CD2	2.48	0.48
1:A:5:GLY:HA2	1:A:35:MET:O	2.12	0.48
1:A:183:ALA:O	1:B:61:ILE:HD13	2.13	0.48
1:D:47:ASP:O	1:D:92:ARG:NH2	2.46	0.48
1:B:1:ILE:HG23	1:B:95:ASP:HB2	1.95	0.48
1:A:288:ASN:CG	1:B:288:ASN:HB3	2.38	0.48
1:B:162:ARG:HH11	1:B:162:ARG:HD2	1.45	0.48
1:A:197:SER:HB3	1:A:200:ASP:HB2	1.96	0.48
1:A:86:ILE:HG23	1:A:117:PHE:HE1	1.78	0.48
1:B:201:LEU:O	1:B:204:GLU:HB2	2.14	0.47
1:B:227:VAL:HG22	2:B:353:HOH:O	2.15	0.47
1:A:125:THR:HG22	1:A:136:THR:HG21	1.95	0.47
1:D:103:ASP:HB2	1:D:300:ILE:HD11	1.95	0.47
1:A:128:ASN:HA	1:A:136:THR:OG1	2.15	0.47
1:A:288:ASN:HB3	1:B:288:ASN:CG	2.39	0.47
1:B:240:ARG:HG2	1:B:240:ARG:NH1	2.24	0.47
1:A:143:LEU:O	1:A:147:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:MET:HA	1:C:115:MET:HE2	1.97	0.47
1:A:7:LEU:HD13	1:A:40:GLY:HA2	1.97	0.47
1:A:114:GLU:C	1:A:116:GLY:H	2.23	0.47
1:C:110:MET:HE3	1:C:114:GLU:HG3	1.97	0.47
1:C:171:ARG:HB3	1:C:223:HIS:HD2	1.79	0.46
1:C:230:LEU:O	1:C:234:ILE:HG13	2.14	0.46
1:C:165:VAL:O	1:C:244:ALA:HA	2.16	0.46
1:D:222:GLU:O	1:D:223:HIS:HB2	2.16	0.46
1:A:82:ARG:HE	1:A:115:MET:HE1	1.80	0.46
1:D:161:GLN:O	1:D:240:ARG:HD2	2.15	0.46
1:A:201:LEU:O	1:A:204:GLU:HB2	2.15	0.46
1:A:1:ILE:HD13	1:A:275:LEU:HB3	1.98	0.46
1:D:110:MET:O	1:D:110:MET:HE3	2.16	0.46
1:B:240:ARG:HH11	1:B:240:ARG:CG	2.22	0.46
1:D:240:ARG:HD3	1:D:240:ARG:HA	1.47	0.46
1:B:45:TYR:HE1	1:B:84:VAL:HG21	1.80	0.46
1:B:206:LYS:HE2	1:B:237:GLU:O	2.16	0.46
1:C:95:ASP:O	1:C:118:PRO:HD2	2.16	0.45
1:A:90:LYS:O	1:A:91:LYS:C	2.58	0.45
1:A:247:LEU:O	1:A:250:ILE:HG12	2.17	0.45
1:B:95:ASP:O	1:B:118:PRO:HD2	2.15	0.45
1:C:210:ALA:C	1:C:212:GLY:H	2.24	0.45
1:A:75:GLU:HB3	1:A:81:ILE:HD13	1.98	0.45
1:A:102:GLY:HA2	1:A:130:ILE:HD11	1.98	0.45
1:A:205:ILE:HG22	1:A:209:ILE:HD12	1.98	0.45
1:C:110:MET:HE2	1:C:297:ILE:HD11	1.97	0.45
1:A:288:ASN:HB3	1:B:288:ASN:CB	2.47	0.45
1:B:77:ARG:O	1:B:82:ARG:NH1	2.50	0.45
1:A:14:PRO:CB	1:A:141:THR:HG21	2.47	0.44
1:B:42:LEU:HD12	1:B:46:GLU:HG3	1.99	0.44
1:C:197:SER:HB3	1:C:200:ASP:OD2	2.17	0.44
1:B:148:GLU:HB2	2:B:390:HOH:O	2.17	0.44
1:B:122:LEU:HD21	1:B:271:ALA:HB2	1.99	0.44
1:B:189:VAL:HA	1:B:219:ALA:O	2.18	0.44
1:A:82:ARG:NE	1:A:115:MET:HE1	2.33	0.44
1:D:240:ARG:HH11	1:D:240:ARG:CG	2.28	0.44
1:C:240:ARG:NH1	1:C:240:ARG:CG	2.68	0.44
1:A:82:ARG:O	1:A:85:ALA:HB3	2.17	0.43
1:B:103:ASP:HB3	1:B:131:LYS:HE2	2.01	0.43
1:C:44:LEU:HD12	1:C:44:LEU:HA	1.84	0.43
1:B:115:MET:HG2	2:B:395:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:LEU:O	1:C:204:GLU:HB2	2.17	0.43
1:D:4:ILE:HG23	1:D:32:LEU:HD13	2.00	0.43
1:A:27:ALA:HA	1:A:32:LEU:HD12	1.99	0.43
1:A:74:PRO:HD2	1:A:75:GLU:OE2	2.19	0.43
1:A:113:THR:HG21	1:A:281:GLY:HA3	2.00	0.43
1:B:214:LYS:H	1:B:214:LYS:HG2	1.70	0.43
1:D:152:ARG:HD2	2:D:361:HOH:O	2.19	0.43
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.90	0.42
1:B:110:MET:HG2	1:B:297:ILE:HD13	1.98	0.42
1:D:102:GLY:HA2	1:D:130:ILE:HD11	2.01	0.42
1:A:19:ALA:HB2	1:A:264:ALA:HB1	2.00	0.42
1:C:152:ARG:HD2	2:C:354:HOH:O	2.19	0.42
1:A:107:MET:HG2	1:A:300:ILE:HD12	2.01	0.42
1:C:252:ARG:NH1	2:C:401:HOH:O	2.47	0.42
1:A:257:VAL:HB	1:A:258:PRO:CD	2.50	0.42
1:C:198:ARG:HH11	1:C:198:ARG:HD3	1.63	0.42
1:D:206:LYS:HG3	1:D:238:THR:HG22	2.02	0.42
1:C:5:GLY:HA3	1:C:97:LEU:HD12	2.00	0.42
1:C:163:ILE:CD1	1:C:240:ARG:HB3	2.50	0.42
1:D:47:ASP:CG	1:D:92:ARG:HH21	2.27	0.42
1:A:45:TYR:CD2	1:A:45:TYR:C	2.98	0.42
1:D:110:MET:SD	1:D:297:ILE:HD11	2.60	0.42
1:A:8:THR:HA	1:A:100:ILE:O	2.21	0.41
1:D:13:ALA:HA	1:D:14:PRO:HD3	1.92	0.41
1:D:122:LEU:HD21	1:D:271:ALA:HB2	2.02	0.41
1:C:113:THR:OG1	1:C:119:CYS:HB2	2.20	0.41
1:C:257:VAL:O	1:C:261:ARG:HG3	2.20	0.41
1:C:5:GLY:CA	1:C:97:LEU:HD12	2.50	0.41
1:B:86:ILE:O	1:B:90:LYS:HB2	2.20	0.41
1:A:187:GLU:HB2	1:A:188:PHE:CE2	2.55	0.41
1:C:51:GLN:NE2	2:C:368:HOH:O	2.49	0.41
1:C:163:ILE:O	1:C:242:THR:HA	2.21	0.41
1:B:17:ASN:HB3	1:B:60:MET:HB3	2.01	0.41
1:B:113:THR:HA	1:B:117:PHE:O	2.21	0.41
1:A:82:ARG:HE	1:A:115:MET:HE3	1.83	0.41
1:B:165:VAL:O	1:B:244:ALA:HA	2.20	0.41
1:B:91:LYS:O	1:B:91:LYS:HG2	2.21	0.41
1:B:171:ARG:HG3	1:B:223:HIS:CD2	2.56	0.41
1:B:231:ALA:HB1	1:B:242:THR:HG22	2.02	0.41
1:A:80:ASN:O	1:A:83:ALA:HB3	2.21	0.40
1:A:288:ASN:CB	1:B:288:ASN:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:VAL:HG21	1:B:233:PHE:HE2	1.82	0.40
1:A:297:ILE:H	1:A:297:ILE:HG13	1.52	0.40
1:B:297:ILE:H	1:B:297:ILE:HG12	1.72	0.40
1:D:28:LEU:HD23	1:D:54:ARG:HG2	2.04	0.40
1:D:224:MET:HE2	1:D:224:MET:HB3	1.95	0.40
1:A:190:VAL:HB	1:A:220:ILE:HG13	2.03	0.40
1:C:122:LEU:HD11	1:C:268:GLY:HA2	2.04	0.40
1:C:154:ARG:O	1:C:158:SER:HB2	2.22	0.40

All (3) 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)
2:D:389:HOH:O	2:D:389:HOH:O[4_556]	1.95	0.25
1:C:236:LYS:NZ	1:D:232:HIS:CD2[4_546]	2.07	0.13
1:A:279:TYR:OH	1:C:87:GLU:OE2[4_556]	2.10	0.10

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	299/320 (93%)	288 (96%)	10 (3%)	1 (0%)	36	50
1	B	299/320 (93%)	293 (98%)	6 (2%)	0	100	100
1	C	300/320 (94%)	292 (97%)	8 (3%)	0	100	100
1	D	303/320 (95%)	290 (96%)	13 (4%)	0	100	100
All	All	1201/1280 (94%)	1163 (97%)	37 (3%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	MET

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	233/255 (91%)	211 (91%)	22 (9%)	8	13
1	B	227/255 (89%)	205 (90%)	22 (10%)	8	12
1	C	233/255 (91%)	215 (92%)	18 (8%)	12	20
1	D	236/255 (92%)	216 (92%)	20 (8%)	10	16
All	All	929/1020 (91%)	847 (91%)	82 (9%)	9	15

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	A	61	ILE
1	A	63	ARG
1	A	66	THR
1	A	77	ARG
1	A	79	GLU
1	A	97	LEU
1	A	103	ASP
1	A	111	ARG
1	A	148	GLU
1	A	162	ARG
1	A	166	VAL
1	A	187	GLU
1	A	202	VAL
1	A	204	GLU
1	A	209	ILE
1	A	214	LYS
1	A	217	ILE
1	A	240	ARG
1	A	241	GLU
1	A	286	ILE

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Mol	Chain	Res	Type
1	A	290	GLN
1	B	0	MET
1	B	4	ILE
1	B	28	LEU
1	B	42	LEU
1	B	49	MET
1	B	56	SER
1	B	61	ILE
1	B	63	ARG
1	B	75	GLU
1	B	81	ILE
1	B	86	ILE
1	B	97	LEU
1	B	107	MET
1	B	111	ARG
1	B	131	LYS
1	B	158	SER
1	B	166	VAL
1	B	187	GLU
1	B	214	LYS
1	B	240	ARG
1	B	286	ILE
1	B	297	ILE
1	C	1	ILE
1	C	28	LEU
1	C	29	THR
1	C	49	MET
1	C	51	GLN
1	C	59	ASP
1	C	63	ARG
1	C	75	GLU
1	C	78	ASP
1	C	81	ILE
1	C	97	LEU
1	C	148	GLU
1	C	158	SER
1	C	166	VAL
1	C	198	ARG
1	C	202	VAL
1	C	240	ARG
1	C	290	GLN
1	D	3	LYS

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Mol	Chain	Res	Type
1	D	28	LEU
1	D	56	SER
1	D	63	ARG
1	D	66	THR
1	D	81	ILE
1	D	91	LYS
1	D	115	MET
1	D	131	LYS
1	D	158	SER
1	D	171	ARG
1	D	178	LEU
1	D	187	GLU
1	D	209	ILE
1	D	236	LYS
1	D	240	ARG
1	D	286	ILE
1	D	298	ASP
1	D	300	ILE
1	D	304	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	160	HIS
1	A	161	GLN
1	A	249	HIS
1	A	294	HIS
1	B	160	HIS
1	B	161	GLN
1	B	232	HIS
1	B	288	ASN
1	C	160	HIS
1	C	161	GLN
1	C	223	HIS
1	C	232	HIS
1	C	288	ASN
1	D	160	HIS
1	D	161	GLN
1	D	223	HIS
1	D	232	HIS
1	D	288	ASN

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Mol	Chain	Res	Type
1	D	294	HIS
1	D	302	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](#)

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.