



Full wwPDB X-ray Structure Validation Report ⓘ

May 31, 2018 – 07:25 PM EDT

PDB ID : 2PFK
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

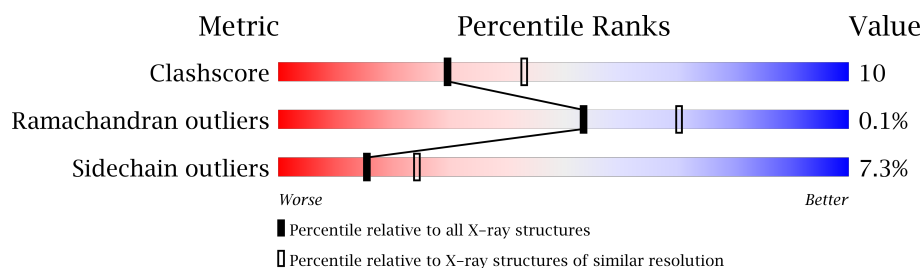
1 Overall quality at a glance

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	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

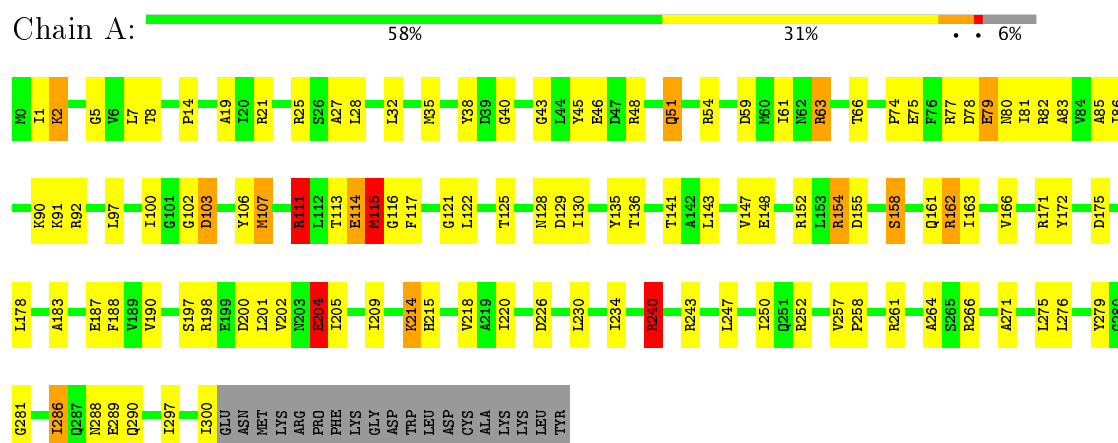
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	81	Total	O	0	0
			81	81		
2	B	76	Total	O	0	0
			76	76		
2	C	94	Total	O	0	0
			94	94		
2	D	96	Total	O	0	0
			96	96		

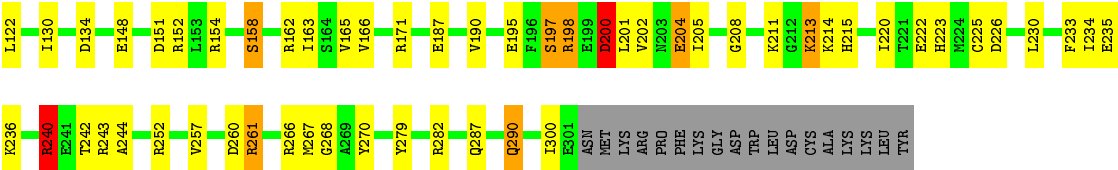
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

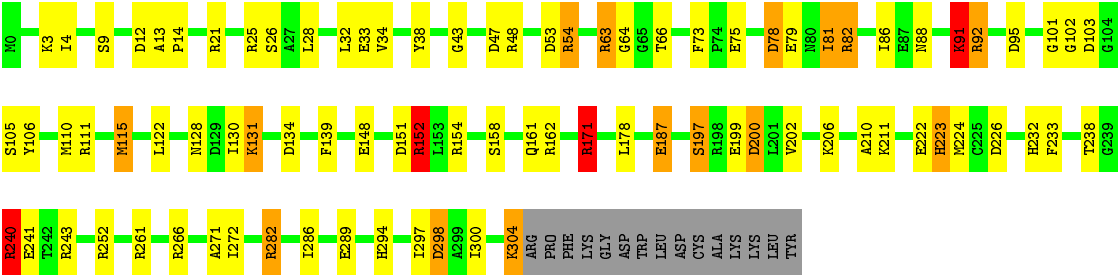
Note EDS was not executed.

• Molecule 1: 6-PHOSPHOFRUCTOKINASE ISOZYME I





• Molecule 1: 6-PHOSPHOFRUCTOKINASE ISOZYME I



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	177.00 Å 66.40 Å 154.00 Å 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	0.84	0/2286	1.95	48/3085 (1.6%)
1	B	0.83	0/2264	1.92	49/3057 (1.6%)
1	C	0.86	0/2282	1.89	55/3081 (1.8%)
1	D	0.84	0/2317	1.92	69/3128 (2.2%)
All	All	0.84	0/9149	1.92	221/12351 (1.8%)

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

There are no bond length outliers.

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ARG	CD-NE-CZ	22.66	155.32	123.60
1	D	243	ARG	NE-CZ-NH1	20.52	130.56	120.30
1	B	152	ARG	CD-NE-CZ	20.30	152.02	123.60
1	A	152	ARG	NE-CZ-NH2	-19.54	110.53	120.30
1	B	152	ARG	NE-CZ-NH2	-18.16	111.22	120.30
1	D	63	ARG	NE-CZ-NH1	16.84	128.72	120.30
1	A	152	ARG	NE-CZ-NH1	15.31	127.96	120.30
1	B	152	ARG	NE-CZ-NH1	14.49	127.54	120.30
1	A	154	ARG	NE-CZ-NH2	-14.41	113.09	120.30
1	A	243	ARG	NE-CZ-NH1	14.38	127.49	120.30
1	D	171	ARG	NE-CZ-NH1	13.39	127.00	120.30
1	C	54	ARG	NE-CZ-NH1	13.18	126.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	152	ARG	NE-CZ-NH2	-12.85	113.87	120.30
1	B	162	ARG	NE-CZ-NH1	-12.82	113.89	120.30
1	C	243	ARG	NE-CZ-NH1	12.60	126.60	120.30
1	B	151	ASP	CB-CG-OD1	12.18	129.26	118.30
1	D	243	ARG	CD-NE-CZ	11.88	140.24	123.60
1	C	282	ARG	NE-CZ-NH1	11.87	126.24	120.30
1	D	25	ARG	NE-CZ-NH2	-11.61	114.50	120.30
1	B	25	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	D	162	ARG	CD-NE-CZ	11.43	139.60	123.60
1	A	240	ARG	NE-CZ-NH2	-11.35	114.63	120.30
1	C	21	ARG	NE-CZ-NH1	11.19	125.89	120.30
1	C	187	GLU	OE1-CD-OE2	-11.13	109.94	123.30
1	B	21	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	D	252	ARG	NE-CZ-NH2	10.91	125.76	120.30
1	A	243	ARG	NE-CZ-NH2	-10.88	114.86	120.30
1	B	21	ARG	NE-CZ-NH2	-10.77	114.92	120.30
1	C	79	GLU	CA-CB-CG	10.61	136.75	113.40
1	A	129	ASP	CB-CG-OD2	-10.56	108.80	118.30
1	D	63	ARG	NE-CZ-NH2	-10.55	115.03	120.30
1	D	243	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	C	21	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	D	82	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	B	243	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	C	39	ASP	CB-CG-OD1	9.74	127.06	118.30
1	D	54	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	C	111	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	D	154	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	C	54	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	A	21	ARG	NE-CZ-NH1	9.15	124.87	120.30
1	A	111	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	C	266	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	D	91	LYS	CA-CB-CG	9.05	133.31	113.40
1	B	25	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	D	48	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	B	92	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	B	243	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	C	211	LYS	C-N-CA	8.80	140.77	122.30
1	D	200	ASP	CB-CG-OD2	-8.70	110.47	118.30
1	A	154	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	C	80	ASN	CB-CA-C	8.54	127.49	110.40
1	B	151	ASP	CB-CG-OD2	-8.52	110.63	118.30
1	D	197	SER	N-CA-CB	8.50	123.25	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	A	51	GLN	CA-CB-CG	8.34	131.75	113.40
1	C	225	CYS	CB-CA-C	-8.29	93.83	110.40
1	A	198	ARG	CA-CB-CG	8.27	131.60	113.40
1	C	261	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	103	ASP	CA-CB-CG	8.06	131.14	113.40
1	C	243	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	B	295	ASP	CB-CG-OD1	7.88	125.39	118.30
1	D	199	GLU	CB-CA-C	7.87	126.15	110.40
1	D	199	GLU	OE1-CD-OE2	-7.78	113.96	123.30
1	A	175	ASP	CB-CG-OD1	7.73	125.26	118.30
1	C	54	ARG	CD-NE-CZ	7.69	134.36	123.60
1	A	155	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	A	152	ARG	CG-CD-NE	-7.62	95.79	111.80
1	D	78	ASP	CB-CG-OD1	7.58	125.13	118.30
1	B	111	ARG	NE-CZ-NH2	7.53	124.06	120.30
1	C	82	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	B	48	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	A	158	SER	N-CA-CB	-7.48	99.28	110.50
1	A	240	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	C	111	ARG	CG-CD-NE	7.32	127.17	111.80
1	D	154	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	D	187	GLU	CB-CG-CD	7.16	133.54	114.20
1	D	261	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	B	106	TYR	CB-CG-CD1	7.15	125.29	121.00
1	D	106	TYR	CB-CG-CD1	7.12	125.27	121.00
1	A	2	LYS	CA-CB-CG	7.10	129.01	113.40
1	A	252	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	A	115	MET	C-N-CA	7.01	137.03	122.30
1	A	92	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	162	ARG	CD-NE-CZ	6.98	133.37	123.60
1	A	135	TYR	CB-CG-CD2	-6.94	116.83	121.00
1	D	266	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	D	226	ASP	N-CA-C	-6.93	92.30	111.00
1	D	199	GLU	CG-CD-OE1	6.92	132.14	118.30
1	D	21	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	78	ASP	CB-CG-OD1	6.91	124.52	118.30
1	C	260	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	C	200	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	D	171	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	C	187	GLU	CG-CD-OE1	6.82	131.95	118.30
1	B	260	ASP	CB-CG-OD1	6.82	124.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	226	ASP	CB-CG-OD2	6.80	124.42	118.30
1	B	59	ASP	N-CA-CB	-6.70	98.53	110.60
1	A	48	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	B	12	ASP	CB-CG-OD2	-6.59	112.36	118.30
1	D	240	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	C	222	GLU	CG-CD-OE2	-6.54	105.22	118.30
1	D	226	ASP	CB-CG-OD2	6.46	124.11	118.30
1	A	158	SER	CB-CA-C	6.44	122.34	110.10
1	A	243	ARG	CD-NE-CZ	6.39	132.54	123.60
1	D	79	GLU	CA-CB-CG	6.38	127.44	113.40
1	D	53	ASP	CB-CG-OD2	6.36	124.03	118.30
1	C	266	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	D	78	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	C	73	PHE	CB-CG-CD2	-6.29	116.39	120.80
1	D	111	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	79	GLU	CA-CB-CG	6.23	127.10	113.40
1	C	225	CYS	O-C-N	6.22	132.65	122.70
1	C	106	TYR	CB-CG-CD1	6.21	124.72	121.00
1	B	231	ALA	CB-CA-C	6.19	119.38	110.10
1	D	162	ARG	CB-CA-C	-6.16	98.08	110.40
1	B	198	ARG	C-N-CA	6.15	137.07	121.70
1	C	282	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	D	25	ARG	NH1-CZ-NH2	6.14	126.16	119.40
1	C	204	GLU	OE1-CD-OE2	6.13	130.65	123.30
1	B	162	ARG	NH1-CZ-NH2	6.10	126.11	119.40
1	D	152	ARG	CG-CD-NE	-6.07	99.06	111.80
1	D	171	ARG	CD-NE-CZ	6.06	132.08	123.60
1	C	25	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	D	199	GLU	CB-CG-CD	6.01	130.43	114.20
1	D	211	LYS	C-N-CA	6.00	134.89	122.30
1	C	279	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	A	226	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	213	LYS	CA-CB-CG	5.97	126.53	113.40
1	C	267	MET	CG-SD-CE	5.97	109.75	100.20
1	B	294	HIS	CB-CA-C	-5.97	98.47	110.40
1	D	134	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	B	175	ASP	CB-CG-OD1	5.91	123.61	118.30
1	A	51	GLN	CB-CA-C	5.86	122.11	110.40
1	B	106	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	A	46	GLU	CG-CD-OE2	-5.78	106.74	118.30
1	D	304	LYS	CA-C-O	5.74	132.16	120.10
1	B	166	VAL	CB-CA-C	-5.71	100.55	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	GLU	OE1-CD-OE2	5.69	130.13	123.30
1	B	47	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	B	152	ARG	CG-CD-NE	-5.67	99.88	111.80
1	D	151	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	73	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	B	226	ASP	N-CA-C	-5.66	95.71	111.00
1	D	224	MET	CA-CB-CG	-5.64	103.70	113.30
1	C	287	GLN	N-CA-CB	5.64	120.75	110.60
1	C	151	ASP	CB-CG-OD1	5.63	123.36	118.30
1	D	33	GLU	OE1-CD-OE2	5.62	130.04	123.30
1	A	204	GLU	OE1-CD-OE2	5.61	130.03	123.30
1	D	73	PHE	CA-CB-CG	5.59	127.31	113.90
1	B	289	GLU	OE1-CD-OE2	5.57	129.99	123.30
1	B	195	GLU	N-CA-CB	5.57	120.62	110.60
1	A	266	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	226	ASP	N-CA-C	-5.55	96.02	111.00
1	D	298	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	D	54	ARG	CB-CA-C	-5.53	99.34	110.40
1	C	235	GLU	CG-CD-OE1	5.51	129.32	118.30
1	A	215	HIS	CA-C-O	5.51	131.66	120.10
1	C	226	ASP	N-CA-C	-5.49	96.17	111.00
1	D	92	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	C	134	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	A	97	LEU	N-CA-CB	-5.47	99.46	110.40
1	C	197	SER	N-CA-CB	5.46	118.70	110.50
1	D	95	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	B	240	ARG	CG-CD-NE	5.44	123.23	111.80
1	C	282	ARG	CD-NE-CZ	5.43	131.20	123.60
1	C	103	ASP	CB-CA-C	5.42	121.25	110.40
1	A	114	GLU	CA-C-N	5.42	129.12	117.20
1	D	12	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	46	GLU	CG-CD-OE1	5.42	129.13	118.30
1	D	289	GLU	CG-CD-OE1	5.41	129.12	118.30
1	B	166	VAL	CG1-CB-CG2	5.41	119.55	110.90
1	B	135	TYR	CB-CG-CD1	-5.41	117.76	121.00
1	C	111	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	D	92	ARG	CD-NE-CZ	5.38	131.14	123.60
1	B	237	GLU	OE1-CD-OE2	5.37	129.75	123.30
1	D	187	GLU	CA-CB-CG	5.37	125.22	113.40
1	B	226	ASP	N-CA-CB	5.36	120.25	110.60
1	C	233	PHE	CB-CG-CD1	-5.36	117.05	120.80
1	B	204	GLU	CG-CD-OE2	-5.36	107.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	CYS	CA-CB-SG	-5.35	104.37	114.00
1	A	63	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	D	64	GLY	C-N-CA	5.33	133.50	122.30
1	C	59	ASP	CB-CA-C	5.32	121.03	110.40
1	A	121	GLY	O-C-N	5.31	131.20	122.70
1	D	162	ARG	CG-CD-NE	-5.30	100.68	111.80
1	D	82	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	106	TYR	CB-CG-CD1	5.29	124.17	121.00
1	C	290	GLN	N-CA-CB	5.27	120.09	110.60
1	B	86	ILE	CB-CA-C	5.27	122.14	111.60
1	B	283	CYS	CB-CA-C	5.27	120.93	110.40
1	A	135	TYR	CB-CG-CD1	5.22	124.13	121.00
1	D	210	ALA	C-N-CA	5.22	134.75	121.70
1	C	1	ILE	N-CA-C	-5.20	96.95	111.00
1	B	3	LYS	CB-CA-C	-5.19	100.03	110.40
1	B	125	THR	CA-CB-CG2	5.18	119.65	112.40
1	D	223	HIS	CA-CB-CG	-5.18	104.80	113.60
1	B	75	GLU	CA-CB-CG	5.17	124.78	113.40
1	A	178	LEU	CB-CA-C	5.17	120.03	110.20
1	C	54	ARG	CA-CB-CG	5.17	124.78	113.40
1	D	148	GLU	CB-CA-C	5.17	120.74	110.40
1	D	131	LYS	CA-CB-CG	5.16	124.76	113.40
1	D	162	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	282	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	D	34	VAL	CA-CB-CG2	5.11	118.57	110.90
1	D	92	ARG	CG-CD-NE	-5.11	101.07	111.80
1	C	63	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	D	241	GLU	OE1-CD-OE2	5.10	129.43	123.30
1	D	21	ARG	CD-NE-CZ	5.10	130.74	123.60
1	A	266	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	195	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	A	103	ASP	N-CA-CB	5.09	119.76	110.60
1	B	222	GLU	CG-CD-OE2	-5.09	108.12	118.30
1	C	117	PHE	O-C-N	5.08	130.76	121.10
1	C	270	TYR	CB-CG-CD1	5.08	124.05	121.00
1	B	212	GLY	N-CA-C	5.07	125.78	113.10
1	C	240	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	D	53	ASP	CB-CG-OD1	-5.07	113.74	118.30
1	B	175	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	B	21	ARG	CD-NE-CZ	5.01	130.61	123.60
1	C	130	ILE	O-C-N	5.01	130.72	122.70

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	57	1
1	B	2233	0	2212	66	0
1	C	2251	0	2239	35	2
1	D	2285	0	2262	32	1
2	A	81	0	0	1	0
2	B	76	0	0	4	0
2	C	94	0	0	4	0
2	D	96	0	0	2	1
All	All	9371	0	8963	183	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 10.

All (183) 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:HD2	1:B:131:LYS:H	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:N	1:B:131:LYS:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:82:ARG:HE	1:A:115:MET:HE3	1.56	0.68
1:C:208:GLY:O	1:C:213:LYS:HB3	1.95	0.68
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:131:LYS:CD	1:B:131:LYS:H	1.96	0.65
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:NH1	1:D:240:ARG:HG2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:82:ARG:HH21	1:B:115:MET:HE1	1.73	0.53
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
1:A:288:ASN:HB3	1:B:288:ASN:HB3	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:C:110:MET:HE3	1:C:114:GLU:HG3	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: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: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:115:MET:HE3	1:D:115:MET:HA	1.93	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:35:MET:HE3	1:B:49:MET:HB2	1.96	0.47
1:A:7:LEU:HD13	1:A:40:GLY:HA2	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: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: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:206:LYS:HE2	1:B:237:GLU:O	2.16	0.46
1:B:45:TYR:HE1	1:B:84:VAL:HG21	1.80	0.46
1:C:95:ASP:O	1:C:118:PRO:HD2	2.16	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: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:A:75:GLU:HB3	1:A:81:ILE:HD13	1.98	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:D:240:ARG:CG	1:D:240:ARG:HH11	2.28	0.44
1:C:240:ARG:CG	1:C:240:ARG:NH1	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
1:C:201:LEU:O	1:C:204:GLU:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:113:THR:HG21	1:A:281:GLY:HA3	2.00	0.43
1:A:74:PRO:HD2	1:A:75:GLU:OE2	2.19	0.43
1:A:288:ASN:CG	1:B:288:ASN:HB3	2.38	0.43
1:B:214:LYS:HG2	1:B:214:LYS:H	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:A:90:LYS:O	1:A:91:LYS:C	2.58	0.42
1:A:288:ASN:HB3	1:B:288:ASN:CG	2.39	0.42
1:C:198:ARG:HD3	1:C:198:ARG:HH11	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: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:163:ILE:O	1:C:242:THR:HA	2.21	0.41
1:C:51:GLN:NE2	2:C:368:HOH:O	2.49	0.41
1:B:113:THR:HA	1:B:117:PHE:O	2.21	0.41
1:B:17:ASN:HB3	1:B:60:MET:HB3	2.01	0.41
1:B:165:VAL:O	1:B:244:ALA:HA	2.20	0.41
1:B:171:ARG:HG3	1:B:223:HIS:CD2	2.56	0.41
1:B:91:LYS:O	1:B:91:LYS:HG2	2.21	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:B:202:VAL:HG21	1:B:233:PHE:HE2	1.82	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:A:297:ILE:HG13	1:A:297:ILE:H	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:A:190:VAL:HB	1:A:220:ILE:HG13	2.03	0.40
1:C:35:MET:HE3	1:C:49:MET:HB2	2.03	0.40
1:C:154:ARG:O	1:C:158:SER:HB2	2.22	0.40
1:C:122:LEU:HD11	1:C:268:GLY:HA2	2.04	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%)	43	58
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%)	53	70

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%)	214 (92%)	19 (8%)	12	19
1	B	227/255 (89%)	210 (92%)	17 (8%)	15	23
1	C	233/255 (91%)	216 (93%)	17 (7%)	15	24
1	D	236/255 (92%)	221 (94%)	15 (6%)	19	30
All	All	929/1020 (91%)	861 (93%)	68 (7%)	15	24

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
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	103	ASP
1	A	107	MET
1	A	111	ARG
1	A	148	GLU
1	A	162	ARG
1	A	166	VAL
1	A	202	VAL
1	A	204	GLU
1	A	214	LYS
1	A	240	ARG
1	A	286	ILE
1	A	290	GLN
1	B	0	MET
1	B	4	ILE
1	B	28	LEU
1	B	42	LEU
1	B	49	MET

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Mol	Chain	Res	Type
1	B	56	SER
1	B	61	ILE
1	B	63	ARG
1	B	75	GLU
1	B	86	ILE
1	B	111	ARG
1	B	131	LYS
1	B	158	SER
1	B	166	VAL
1	B	214	LYS
1	B	240	ARG
1	B	286	ILE
1	C	28	LEU
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	200	ASP
1	C	202	VAL
1	C	240	ARG
1	C	290	GLN
1	D	3	LYS
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	240	ARG
1	D	286	ILE

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Mol	Chain	Res	Type
1	D	298	ASP
1	D	304	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	161	GLN
1	B	161	GLN
1	B	223	HIS
1	B	232	HIS
1	B	288	ASN
1	C	161	GLN
1	C	223	HIS
1	C	288	ASN
1	D	161	GLN
1	D	223	HIS
1	D	302	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.