



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:26 AM UTC

PDB ID : 1BBR / pdb_00001bbr
Title : THE STRUCTURE OF RESIDUES 7-16 OF THE A ALPHA CHAIN
OF HUMAN FIBRINOGEN BOUND TO BOVINE THROMBIN AT 2.3
ANGSTROMS RESOLUTION
Authors : Martin, P.; Edwards, B.
Deposited on : 1992-04-27
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

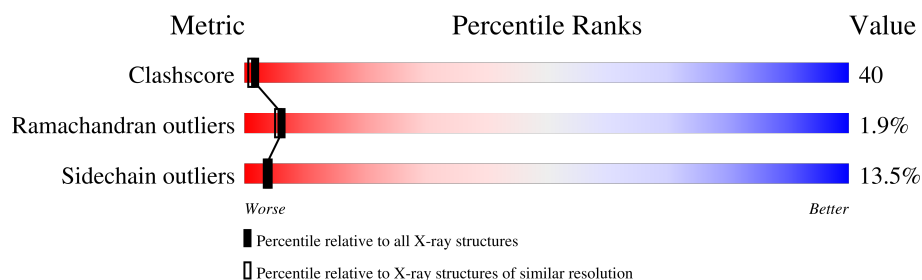
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	J	49	22% 35% 14% • 27%
1	L	49	29% 33% 10% • 27%
1	M	49	16% 45% 12% 27%
2	H	150	36% 43% 14% 7%
3	E	109	40% 38% 18% •
4	F	11	27% 45% 18% 9%
4	G	11	55% 18% 27%
4	I	11	36% 55% 9%

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Mol	Chain	Length	Quality of chain
5	K	259	35% 36% 23% 6%
5	N	259	34% 47% 17%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8084 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 EPSILON-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	36	Total	C	N	O	S	0	0	0
			290	181	48	60	1			
1	J	36	Total	C	N	O	S	0	0	0
			290	181	48	60	1			
1	M	36	Total	C	N	O	S	0	0	0
			290	181	48	60	1			

- Molecule 2 is a protein called EPSILON-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	150	Total	C	N	O	S	0	0	0
			1235	793	222	215	5			

- Molecule 3 is a protein called EPSILON-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	109	Total	C	N	O	S	0	0	0
			860	544	154	155	7			

- Molecule 4 is a protein called FIBRINOGEN ALPHA/ALPHA-E CHAIN PRECURSOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	11	Total	C	N	O	0	0	0
			75	46	13	16			
4	G	11	Total	C	N	O	0	0	0
			75	46	13	16			
4	I	11	Total	C	N	O	0	0	0
			75	46	13	16			

- Molecule 5 is a protein called EPSILON-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	259	Total 2094	C 1337	N 376	O 369	S 12	0	0	0
5	N	259	Total 2094	C 1337	N 376	O 369	S 12	0	0	0

- Molecule 6 is water.

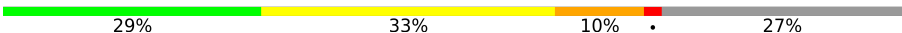
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	31	Total 31	O 31	0	0
6	H	126	Total 126	O 126	0	0
6	E	69	Total 69	O 69	0	0
6	F	10	Total 10	O 10	0	0
6	J	23	Total 23	O 23	0	0
6	K	213	Total 213	O 213	0	0
6	G	11	Total 11	O 11	0	0
6	M	26	Total 26	O 26	0	0
6	N	188	Total 188	O 188	0	0
6	I	9	Total 9	O 9	0	0

3 Residue-property plots [i](#)

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.

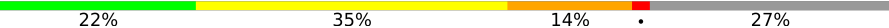
Note EDS was not executed.

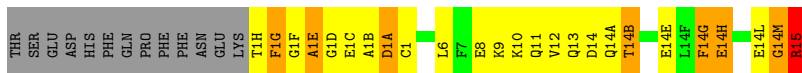
• Molecule 1: EPSILON-THROMBIN

Chain L: 



• Molecule 1: EPSILON-THROMBIN

Chain J: 

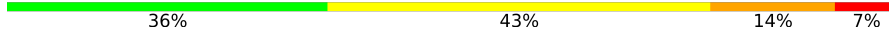


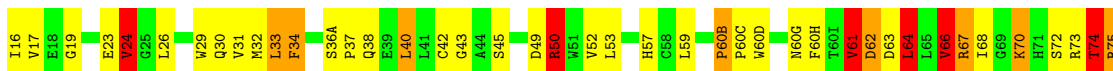
• Molecule 1: EPSILON-THROMBIN

Chain M: 

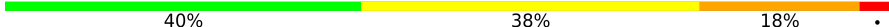


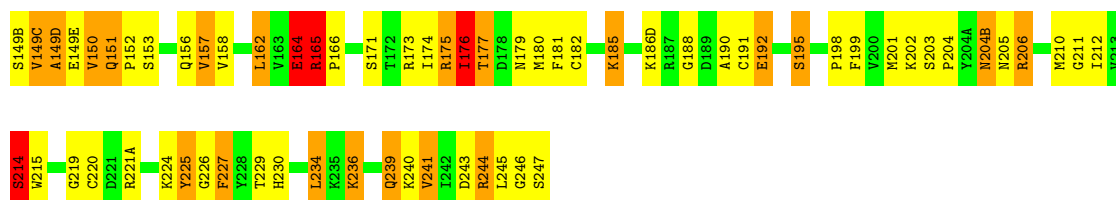
• Molecule 2: EPSILON-THROMBIN

Chain H: 



• Molecule 3: EPSILON-THROMBIN

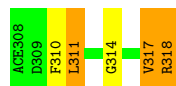
Chain E: 



• Molecule 4: FIBRINOGEN ALPHA/ALPHA-E CHAIN PRECURSOR



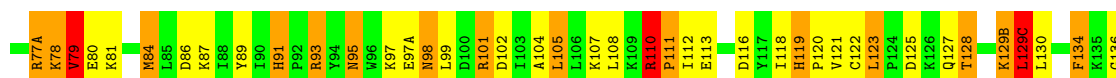
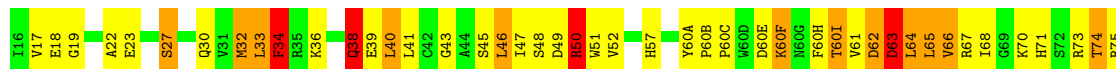
• Molecule 4: FIBRINOGEN ALPHA/ALPHA-E CHAIN PRECURSOR



• Molecule 4: FIBRINOGEN ALPHA/ALPHA-E CHAIN PRECURSOR



• Molecule 5: EPSILON-THROMBIN



• Molecule 5: EPSILON-THROMBIN



V200	T139	S80	I16
M201	G140	K81	V17
K202	W141	I82	E23
S203	G142	S83	V24
P204	N143	M84	G25
Y204A	R144	L85	L26
N204B		D86	S27
N205	T147	K87	W29
R206	W148	I88	
R207	T149	Y89	L33
Y208	T149A	I90	F34
Q209	S149B	H91	R35
W210	Y149C	P92	
G211	A149D	R93	Q38
I212	E149E	Y94	E39
	V150	N95	L40
W215	Q151	M96	
G216	P152	K97	G43
E217	S153	E97A	A44
G219	V154	N98	S45
G220	L155	L99	L46
D221	Q156	D100	I47
R221A	V157	R101	S48
D222	V158	D102	D49
G223	N159	I103	R50
K224			L53
Y225	E164	L106	H57
G226	R165	K107	C58
F227	P166	L108	L59
Y228	V167	K109	G60A
	K168	R110	P60B
F232	K169	P111	P60C
R233	A170	I112	W60D
L234	S171	L114	D60E
K235	T172	S115	K60F
K236	R173	D116	T601
V237	I174	Y117	V61
I238	R175	I118	L84
Q239	I176	H119	L65
K240	T177		V66
V241	D178	C122	R67
L242	F181	L123	I68
D243		P124	
R244	K185	D125	H71
L245	P186	K126	S72
G246	G186A	Q127	R73
S247	E186B	T128	T74
	R187		R75
		K128B	Y76
		L129C	E77
		L130	R77A
	C191	H131	K78
	E192	A132	V79
	G193	G133	
	D194	F134	
	S195	K135	
	G196	G136	
	G197	R137	
	P198	V138	
	F199		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.02Å 89.41Å 99.30Å 90.00° 106.64° 90.00°	Depositor
Resolution (Å)	7.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8084	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE

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	J	1.31	0/294	2.35	14/390 (3.6%)
1	L	1.23	0/294	1.97	8/390 (2.1%)
1	M	1.22	1/294 (0.3%)	2.13	15/390 (3.8%)
2	H	1.45	10/1267 (0.8%)	2.15	47/1716 (2.7%)
3	E	1.46	4/881 (0.5%)	2.19	45/1186 (3.8%)
4	F	1.30	0/73	2.60	6/95 (6.3%)
4	G	1.41	1/73 (1.4%)	2.19	4/95 (4.2%)
4	I	1.50	0/73	2.11	2/95 (2.1%)
5	K	1.67	19/2148 (0.9%)	2.43	147/2905 (5.1%)
5	N	1.40	11/2148 (0.5%)	2.12	80/2905 (2.8%)
All	All	1.48	46/7545 (0.6%)	2.24	368/10167 (3.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
2	H	0	2
3	E	0	2
4	G	0	1
5	K	0	6
5	N	0	5
All	All	0	17

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	19	GLY	N-CA	13.04	1.54	1.44
5	N	33	LEU	N-CA	8.80	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	184	GLY	N-CA	7.69	1.53	1.45
5	N	219	GLY	CA-C	7.37	1.60	1.52
2	H	52	VAL	N-CA	6.87	1.54	1.46
5	K	60(F)	LYS	CA-CB	-6.60	1.44	1.53
5	K	186(B)	GLU	C-O	6.57	1.32	1.24
5	K	43	GLY	N-CA	6.56	1.51	1.44
5	N	157	VAL	N-CA	-6.47	1.38	1.46
5	K	210	MET	N-CA	6.21	1.54	1.46
5	N	74	THR	CA-CB	6.14	1.64	1.53
2	H	103	ILE	CA-CB	6.07	1.63	1.54
5	K	136	GLY	N-CA	6.02	1.50	1.45
3	E	204(B)	ASN	C-O	6.02	1.31	1.23
4	G	317	VAL	N-CA	5.86	1.53	1.46
5	K	210	MET	CA-C	-5.85	1.44	1.52
5	K	149(A)	THR	CA-CB	5.84	1.63	1.53
5	N	98	ASN	C-O	5.78	1.28	1.23
5	K	30	GLN	C-O	5.78	1.30	1.23
2	H	30	GLN	C-O	5.71	1.30	1.24
5	K	74	THR	CA-CB	5.64	1.62	1.53
2	H	62	ASP	N-CA	5.63	1.54	1.46
5	K	77(A)	ARG	C-O	5.63	1.30	1.24
3	E	164	GLU	N-CA	5.63	1.52	1.46
2	H	49	ASP	N-CA	5.58	1.53	1.46
5	K	191	CYS	N-CA	5.54	1.53	1.46
5	N	172	THR	CA-CB	5.53	1.63	1.53
2	H	19	GLY	N-CA	5.52	1.48	1.44
5	N	57	HIS	ND1-CE1	-5.51	1.27	1.32
5	K	212	ILE	CB-CG1	5.50	1.64	1.53
5	K	194	ASP	C-N	-5.44	1.26	1.33
5	K	159	ASN	N-CA	5.43	1.52	1.46
5	K	68	ILE	CA-CB	5.42	1.61	1.54
2	H	147	THR	CA-CB	5.39	1.61	1.53
2	H	26	LEU	N-CA	-5.38	1.39	1.46
5	K	60(A)	TYR	CA-CB	5.38	1.58	1.53
5	N	186(B)	GLU	C-O	5.36	1.30	1.24
5	N	136	GLY	N-CA	5.29	1.49	1.44
5	K	226	GLY	N-CA	5.25	1.52	1.45
5	N	33	LEU	CA-CB	-5.21	1.46	1.53
5	N	64	LEU	CA-CB	5.19	1.62	1.53
3	E	227	PHE	N-CA	5.16	1.52	1.46
1	M	14(M)	GLY	N-CA	-5.13	1.38	1.45
2	H	148	TRP	CA-C	5.11	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	212	ILE	N-CA	-5.09	1.40	1.46
2	H	105	LEU	N-CA	5.05	1.52	1.46

All (368) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	79	VAL	N-CA-C	14.79	127.12	111.00
5	K	134	PHE	CA-CB-CG	13.89	127.69	113.80
5	K	60(F)	LYS	CA-CB-CG	13.78	141.65	114.10
5	K	80	GLU	CB-CG-CD	12.85	134.44	112.60
5	K	186(B)	GLU	N-CA-C	12.43	126.24	111.82
5	N	75	ARG	CD-NE-CZ	12.32	141.65	124.40
5	K	95	ASN	OD1-CG-ND2	-12.19	110.41	122.60
5	N	33	LEU	CB-CA-C	11.18	128.13	109.80
5	K	186(B)	GLU	CA-C-O	-11.02	107.29	119.97
1	J	14(G)	PHE	CA-CB-CG	-10.89	102.91	113.80
5	N	39	GLU	CA-CB-CG	10.70	135.50	114.10
5	N	119	HIS	CA-CB-CG	10.44	124.24	113.80
5	N	74	THR	N-CA-C	9.52	124.43	113.01
1	M	14(M)	GLY	N-CA-C	9.50	135.70	113.18
1	M	1(F)	GLY	N-CA-C	-9.44	102.96	115.32
5	N	79	VAL	N-CA-C	9.37	122.33	112.96
3	E	176	ILE	CB-CA-C	9.24	121.80	111.45
5	N	64	LEU	N-CA-C	9.21	124.41	109.59
5	K	121	VAL	CA-C-O	-9.18	114.43	121.68
5	K	63	ASP	CA-CB-CG	9.04	121.64	112.60
1	J	14(E)	GLU	CB-CG-CD	8.97	127.85	112.60
5	K	51	TRP	CA-C-N	8.97	134.89	123.14
5	K	51	TRP	C-N-CA	8.97	134.89	123.14
1	J	14(H)	GLU	CB-CG-CD	8.90	127.72	112.60
4	G	314	GLY	N-CA-C	8.86	126.73	115.21
1	J	14	ASP	CA-CB-CG	8.76	121.36	112.60
5	K	145	ARG	CA-CB-CG	8.66	131.41	114.10
5	K	146	GLU	CB-CG-CD	8.60	127.21	112.60
5	K	101	ARG	CD-NE-CZ	-8.58	112.38	124.40
5	K	190	ALA	N-CA-C	-8.56	97.85	110.52
3	E	190	ALA	N-CA-C	-8.40	99.69	110.53
5	K	79	VAL	CA-C-O	-8.34	110.36	120.78
5	K	148	TRP	N-CA-C	8.28	118.87	108.19
4	F	314	GLY	N-CA-C	8.18	125.85	115.21
2	H	135	LYS	CA-C-N	8.15	130.12	121.48
2	H	135	LYS	C-N-CA	8.15	130.12	121.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	185	LYS	CA-CB-CG	8.14	130.38	114.10
5	N	157	VAL	CB-CA-C	-8.13	97.68	110.69
5	N	168	CYS	CA-C-N	8.12	131.16	120.28
5	N	168	CYS	C-N-CA	8.12	131.16	120.28
5	N	97(A)	GLU	N-CA-C	8.11	121.30	111.40
5	N	186(B)	GLU	N-CA-C	8.08	128.02	110.80
5	K	77(A)	ARG	N-CA-C	8.05	120.77	111.11
1	L	14(E)	GLU	CB-CG-CD	8.04	126.26	112.60
5	K	39	GLU	N-CA-C	8.00	122.31	110.48
5	K	43	GLY	N-CA-C	-7.95	100.02	112.58
1	M	14	ASP	CA-CB-CG	7.89	120.49	112.60
2	H	100	ASP	CA-C-O	-7.87	112.07	121.05
5	K	161	PRO	O-C-N	7.86	132.53	123.10
5	K	175	ARG	CD-NE-CZ	-7.77	113.53	124.40
2	H	64	LEU	N-CA-C	7.73	120.91	109.24
3	E	198	PRO	CA-C-N	7.73	134.80	123.13
3	E	198	PRO	C-N-CA	7.73	134.80	123.13
3	E	204(B)	ASN	CA-C-O	-7.72	112.23	120.80
2	H	33	LEU	O-C-N	7.71	132.01	123.22
5	K	149	THR	N-CA-CB	7.68	123.46	110.49
1	M	2	GLY	N-CA-C	7.66	125.54	115.36
3	E	158	VAL	CA-C-O	-7.65	112.71	120.90
5	K	190	ALA	CA-C-O	-7.62	112.73	121.72
1	J	1(A)	ASP	CA-CB-CG	-7.60	105.00	112.60
1	J	1(G)	PHE	CA-CB-CG	7.59	121.39	113.80
5	N	181	PHE	CA-C-O	-7.58	112.83	121.40
5	N	164	GLU	CA-CB-CG	7.57	129.24	114.10
5	K	19	GLY	N-CA-C	-7.57	102.37	112.81
5	K	74	THR	N-CA-C	7.54	122.92	112.45
1	M	14(E)	GLU	CB-CG-CD	7.41	125.20	112.60
5	K	110	ARG	O-C-N	7.38	127.12	121.88
5	N	79	VAL	CA-C-O	-7.37	113.10	119.29
5	K	191	CYS	CA-C-O	-7.31	113.61	121.36
5	K	123	LEU	N-CA-C	-7.29	100.25	110.31
5	K	95	ASN	CA-CB-CG	7.28	119.88	112.60
5	K	204(B)	ASN	OD1-CG-ND2	-7.25	115.35	122.60
4	F	317	VAL	N-CA-C	-7.24	100.17	109.80
5	K	93	ARG	N-CA-C	7.21	121.39	112.59
5	N	176	ILE	CB-CA-C	7.20	121.21	111.28
5	K	84	MET	N-CA-C	-7.17	99.85	110.46
5	N	165	ARG	CD-NE-CZ	-7.15	114.38	124.40
2	H	40	LEU	CA-C-O	-7.14	112.21	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	33	LEU	CA-CB-CG	7.11	141.17	116.30
3	E	153	SER	N-CA-C	-7.10	104.77	113.50
5	K	186(B)	GLU	CA-C-N	7.08	130.36	116.20
2	H	23	GLU	CA-C-O	-7.01	113.54	121.81
5	K	80	GLU	CA-CB-CG	7.00	128.11	114.10
1	M	1(G)	PHE	CA-CB-CG	6.98	120.78	113.80
5	N	46	LEU	CA-C-O	-6.97	112.62	120.43
5	K	62	ASP	CA-CB-CG	6.94	119.54	112.60
5	N	216	GLY	CA-C-O	-6.94	114.09	121.38
3	E	211	GLY	CA-C-N	6.94	132.63	122.99
3	E	211	GLY	C-N-CA	6.94	132.63	122.99
5	K	62	ASP	CA-C-N	6.91	134.65	122.42
5	K	62	ASP	C-N-CA	6.91	134.65	122.42
5	K	119	HIS	CA-C-N	6.88	126.80	119.85
5	K	119	HIS	C-N-CA	6.88	126.80	119.85
5	K	102	ASP	CA-C-O	-6.85	114.13	122.41
1	J	13	GLN	CA-C-O	-6.85	113.60	121.47
5	N	143	ASN	CA-CB-CG	6.84	119.44	112.60
3	E	204(B)	ASN	N-CA-C	-6.81	98.59	109.76
2	H	45	SER	CA-C-N	6.80	131.47	122.42
2	H	45	SER	C-N-CA	6.80	131.47	122.42
5	K	159	ASN	CA-C-O	-6.80	113.25	120.80
5	K	225	TYR	CA-C-N	-6.74	112.15	120.64
5	K	225	TYR	C-N-CA	-6.74	112.15	120.64
1	M	13	GLN	CA-C-O	-6.70	113.61	120.71
5	K	139	THR	CA-CB-CG2	6.70	121.88	110.50
5	K	60(E)	ASP	CA-C-O	-6.66	113.36	121.28
2	H	23	GLU	N-CA-C	-6.62	101.61	110.55
5	N	64	LEU	N-CA-CB	-6.62	100.04	110.69
2	H	147	THR	CA-C-N	6.60	134.16	121.54
2	H	147	THR	C-N-CA	6.60	134.16	121.54
1	M	14(G)	PHE	CA-CB-CG	-6.59	107.21	113.80
5	K	212	ILE	CA-CB-CG2	6.56	121.66	110.50
5	K	225	TYR	CB-CG-CD1	6.56	130.63	120.80
5	K	177	THR	CA-CB-OG1	-6.55	99.78	109.60
3	E	162	LEU	CA-CB-CG	6.52	139.12	116.30
5	K	98	ASN	OD1-CG-ND2	-6.51	116.08	122.60
5	K	175	ARG	NE-CZ-NH2	-6.51	113.34	119.20
5	K	239	GLN	OE1-CD-NE2	6.51	129.11	122.60
5	K	77(A)	ARG	CA-C-O	-6.51	113.94	120.90
5	N	209	GLN	O-C-N	6.50	130.86	122.87
1	L	1(A)	ASP	N-CA-C	6.49	121.41	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	167	VAL	N-CA-C	-6.49	103.93	111.00
5	K	151	GLN	O-C-N	6.48	128.51	121.12
3	E	164	GLU	CA-C-N	6.48	131.79	121.62
3	E	164	GLU	C-N-CA	6.48	131.79	121.62
5	K	199	PHE	CA-C-O	-6.45	113.83	120.54
5	K	34	PHE	N-CA-CB	-6.43	99.64	110.83
2	H	24	VAL	CA-C-O	-6.41	114.99	121.59
5	N	60(E)	ASP	CA-C-O	-6.35	114.18	121.54
3	E	230	HIS	CA-C-N	6.34	128.78	120.60
3	E	230	HIS	C-N-CA	6.34	128.78	120.60
5	N	175	ARG	CD-NE-CZ	-6.33	115.54	124.40
5	N	232	PHE	CA-CB-CG	-6.32	107.48	113.80
5	N	84	MET	N-CA-C	-6.30	100.88	110.14
2	H	148	TRP	N-CA-CB	6.29	121.13	110.49
4	F	317	VAL	CA-C-O	-6.28	115.12	121.59
3	E	176	ILE	CA-CB-CG2	6.27	121.17	110.50
5	K	80	GLU	N-CA-C	6.27	119.92	109.95
5	N	123	LEU	N-CA-C	-6.24	100.57	109.62
3	E	190	ALA	N-CA-CB	6.23	119.35	110.44
5	K	23	GLU	CA-C-O	-6.22	114.65	121.87
5	K	229	THR	O-C-N	6.22	130.58	122.93
5	K	178	ASP	CA-CB-CG	-6.21	106.39	112.60
5	K	167	VAL	CA-C-O	-6.19	113.78	120.47
5	N	186(B)	GLU	CA-C-N	6.16	128.53	116.20
5	K	225	TYR	CB-CG-CD2	-6.15	111.58	120.80
5	K	97(A)	GLU	CB-CG-CD	6.14	123.04	112.60
4	F	317	VAL	CB-CA-C	6.12	119.73	111.28
3	E	165	ARG	CD-NE-CZ	-6.12	115.83	124.40
5	K	18	GLU	CB-CA-C	-6.11	101.92	111.39
5	K	105	LEU	CA-C-N	6.11	131.61	123.00
5	K	105	LEU	C-N-CA	6.11	131.61	123.00
5	N	194	ASP	CA-C-O	6.11	125.86	119.14
5	K	77(A)	ARG	CA-CB-CG	6.08	126.27	114.10
5	N	164	GLU	CB-CG-CD	6.08	122.94	112.60
5	K	209	GLN	O-C-N	6.08	130.23	122.93
2	H	50	ARG	N-CA-C	6.07	122.56	114.12
5	K	33	LEU	N-CA-CB	6.06	120.30	110.42
3	E	157	VAL	CB-CA-C	-6.05	101.18	110.50
5	K	67	ARG	CD-NE-CZ	-6.05	115.93	124.40
5	K	234	LEU	CB-CA-C	6.04	120.18	110.09
2	H	147	THR	N-CA-C	6.03	118.95	109.96
5	N	73	ARG	CA-C-N	6.03	133.12	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	73	ARG	C-N-CA	6.03	133.12	121.18
5	K	110	ARG	CB-CA-C	-6.03	98.96	108.91
5	N	234	LEU	CA-C-N	6.02	128.67	120.54
5	N	234	LEU	C-N-CA	6.02	128.67	120.54
5	K	146	GLU	CA-CB-CG	6.01	126.12	114.10
5	N	23	GLU	CA-CB-CG	5.99	126.08	114.10
5	K	148	TRP	CA-CB-CG	5.97	124.95	113.60
5	N	16	ILE	CB-CG1-CD1	5.96	126.31	113.80
2	H	30	GLN	OE1-CD-NE2	-5.94	116.66	122.60
1	L	1(G)	PHE	CA-CB-CG	5.93	119.73	113.80
5	K	196	GLY	CA-C-O	-5.93	113.01	119.59
5	K	74	THR	CA-CB-OG1	-5.93	100.71	109.60
5	N	23	GLU	O-C-N	5.92	130.12	123.19
5	N	86	ASP	CA-CB-CG	-5.91	106.69	112.60
2	H	66	VAL	CB-CA-C	5.91	119.16	110.77
5	K	60(I)	THR	N-CA-CB	5.90	119.50	110.70
5	N	209	GLN	N-CA-CB	5.90	120.13	110.39
3	E	191	CYS	O-C-N	5.89	129.29	122.99
3	E	176	ILE	CA-C-N	5.87	131.72	122.21
3	E	176	ILE	C-N-CA	5.87	131.72	122.21
5	N	43	GLY	N-CA-C	-5.86	101.44	112.10
2	H	148	TRP	N-CA-C	-5.85	98.34	110.80
5	N	157	VAL	N-CA-CB	5.84	122.73	111.93
5	K	157	VAL	CB-CA-C	-5.83	101.06	110.28
5	N	57	HIS	CA-CB-CG	5.83	119.63	113.80
5	K	162	LEU	N-CA-C	-5.80	102.32	110.50
3	E	243	ASP	CA-C-N	5.80	132.62	121.54
3	E	243	ASP	C-N-CA	5.80	132.62	121.54
1	M	14(K)	ILE	CB-CA-C	5.80	118.09	110.84
2	H	75	ARG	N-CA-C	5.79	118.22	110.35
5	K	176	ILE	CA-C-O	-5.78	114.99	121.98
5	N	226	GLY	CA-C-O	-5.77	115.07	121.94
5	K	227	PHE	CA-C-N	5.77	131.60	122.94
5	K	227	PHE	C-N-CA	5.77	131.60	122.94
1	M	11	GLN	CB-CG-CD	5.77	122.41	112.60
1	J	8	GLU	CB-CG-CD	5.77	122.40	112.60
2	H	146	GLU	CB-CA-C	-5.76	101.62	110.26
5	K	235	LYS	N-CA-C	5.75	118.32	111.71
2	H	34	PHE	N-CA-CB	-5.74	100.61	111.00
5	N	209	GLN	CA-C-O	-5.74	114.64	120.84
2	H	62	ASP	CB-CA-C	5.74	120.97	110.36
5	K	148	TRP	CA-C-O	5.73	126.82	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	93	ARG	CA-C-N	5.73	128.97	120.95
5	K	93	ARG	C-N-CA	5.73	128.97	120.95
5	N	144	ARG	CD-NE-CZ	-5.72	116.39	124.40
5	K	229	THR	CA-CB-OG1	-5.72	101.03	109.60
2	H	64	LEU	N-CA-CB	-5.71	101.75	111.69
5	K	212	ILE	CA-C-O	-5.70	114.40	120.39
5	N	60(B)	PRO	CB-CA-C	5.70	117.88	110.92
5	N	89	TYR	CA-C-O	-5.69	114.42	120.40
2	H	19	GLY	N-CA-C	-5.69	104.96	112.81
5	N	34	PHE	CA-CB-CG	5.69	119.49	113.80
5	N	132	ALA	CA-C-O	-5.68	114.90	121.15
5	N	219	GLY	N-CA-C	-5.67	102.35	112.22
5	K	129(C)	LEU	N-CA-C	5.66	120.20	113.12
2	H	38	GLN	OE1-CD-NE2	-5.66	116.94	122.60
2	H	61	VAL	N-CA-CB	-5.66	104.23	110.51
5	N	186(B)	GLU	CA-C-O	-5.65	112.42	120.51
5	K	198	PRO	N-CA-C	5.65	122.83	111.69
5	N	67	ARG	CD-NE-CZ	-5.64	116.50	124.40
5	N	156	GLN	OE1-CD-NE2	5.64	128.24	122.60
3	E	206	ARG	NE-CZ-NH1	-5.64	115.86	121.50
2	H	146	GLU	N-CA-CB	5.63	118.38	109.71
5	N	84	MET	CA-C-O	-5.63	114.58	121.78
3	E	226	GLY	CA-C-O	-5.62	116.47	121.64
5	K	91	HIS	CA-CB-CG	-5.62	108.18	113.80
1	M	4	ARG	N-CA-C	5.62	117.74	109.42
3	E	177	THR	N-CA-CB	-5.62	101.91	111.69
5	K	179	ASN	OD1-CG-ND2	5.62	128.22	122.60
2	H	102	ASP	CA-CB-CG	-5.60	107.00	112.60
5	N	136	GLY	N-CA-C	-5.59	102.78	112.06
3	E	225	TYR	CA-C-N	5.57	127.01	120.71
3	E	225	TYR	C-N-CA	5.57	127.01	120.71
5	K	49	ASP	CA-CB-CG	-5.56	107.04	112.60
3	E	157	VAL	CA-C-O	-5.55	114.45	120.67
5	N	237	TRP	N-CA-C	-5.55	104.74	112.45
1	L	4	ARG	CD-NE-CZ	-5.54	116.64	124.40
5	K	80	GLU	CA-C-O	5.54	127.42	121.16
1	J	14(M)	GLY	N-CA-C	-5.53	105.99	113.24
5	K	98	ASN	CA-C-O	-5.53	113.76	119.51
5	N	199	PHE	N-CA-CB	5.53	119.88	110.87
5	N	212	ILE	CA-C-O	-5.53	114.59	120.39
3	E	181	PHE	CB-CA-C	5.50	121.07	109.79
5	K	168	CYS	CB-CA-C	-5.50	101.51	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	42	CYS	N-CA-CB	-5.47	103.03	111.46
5	K	66	VAL	N-CA-CB	-5.47	101.08	111.21
5	K	235	LYS	CA-C-O	-5.47	113.91	120.10
5	K	145	ARG	CA-C-O	-5.47	114.62	120.75
5	N	65	LEU	CA-C-O	-5.47	114.93	121.11
2	H	43	GLY	N-CA-C	-5.47	103.16	112.51
2	H	74	THR	CA-CB-OG1	-5.46	101.40	109.60
5	N	61	VAL	CA-C-O	-5.46	114.69	120.64
1	M	13	GLN	O-C-N	5.46	130.14	123.21
5	K	199	PHE	N-CA-C	-5.45	98.88	108.20
5	K	150	VAL	CB-CA-C	5.45	120.23	111.29
1	J	9	LYS	CA-C-N	5.43	132.21	122.38
1	J	9	LYS	C-N-CA	5.43	132.21	122.38
2	H	99	LEU	O-C-N	5.43	128.81	122.67
1	M	14(L)	GLU	N-CA-C	-5.43	101.61	109.59
5	K	211	GLY	CA-C-N	5.42	130.25	123.14
5	K	211	GLY	C-N-CA	5.42	130.25	123.14
5	K	27	SER	N-CA-CB	-5.42	104.37	111.09
2	H	52	VAL	CA-C-O	-5.42	114.33	120.67
5	N	220	CYS	CA-C-O	-5.41	114.10	120.60
5	K	205	ASN	CA-CB-CG	-5.41	107.19	112.60
2	H	80	GLU	CA-CB-CG	5.39	124.88	114.10
5	N	83	SER	N-CA-CB	5.39	120.00	111.43
5	K	204(B)	ASN	CA-CB-CG	5.38	117.98	112.60
5	K	50	ARG	CD-NE-CZ	5.38	131.93	124.40
5	K	142	GLY	CA-C-N	5.37	129.32	121.31
5	K	142	GLY	C-N-CA	5.37	129.32	121.31
5	N	141	TRP	CA-C-N	5.37	128.04	121.06
5	N	141	TRP	C-N-CA	5.37	128.04	121.06
5	K	97(A)	GLU	CA-CB-CG	5.36	124.82	114.10
5	K	129(C)	LEU	N-CA-CB	-5.36	102.23	110.42
1	J	14(E)	GLU	CA-CB-CG	5.35	124.81	114.10
4	G	317	VAL	N-CA-C	-5.35	102.68	109.58
3	E	199	PHE	CA-C-N	-5.35	114.75	122.45
3	E	199	PHE	C-N-CA	-5.35	114.75	122.45
5	N	48	SER	CA-C-O	-5.34	115.64	121.14
5	K	64	LEU	N-CA-C	5.34	117.53	109.41
1	L	14(C)	GLU	CA-CB-CG	5.32	124.75	114.10
5	K	149(E)	GLU	N-CA-CB	5.31	119.73	110.81
2	H	123	LEU	CB-CA-C	5.30	115.83	109.31
5	K	194	ASP	CA-C-O	-5.30	112.87	119.18
5	K	205	ASN	OD1-CG-ND2	5.30	127.91	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	32	MET	CA-C-N	5.29	129.81	122.77
5	K	32	MET	C-N-CA	5.29	129.81	122.77
5	K	134	PHE	CB-CA-C	5.29	118.47	109.53
5	K	206	ARG	O-C-N	5.29	129.18	123.10
5	K	229	THR	N-CA-CB	5.28	117.72	109.85
1	M	4	ARG	CA-C-O	5.27	123.52	119.46
5	N	119	HIS	CB-CA-C	5.27	117.38	109.63
3	E	162	LEU	CB-CA-C	5.25	118.29	109.89
2	H	103	ILE	O-C-N	5.25	129.18	123.09
2	H	60(B)	PRO	N-CA-C	5.24	117.09	110.70
5	K	224	LYS	CA-C-O	-5.24	115.27	121.66
5	K	63	ASP	CA-C-O	5.24	125.61	119.06
5	K	111	PRO	N-CA-C	-5.24	103.06	111.38
5	K	137	ARG	CB-CA-C	5.23	119.37	109.37
5	K	189	ASP	CB-CA-C	5.23	121.43	111.17
5	K	219	GLY	N-CA-C	-5.23	103.11	112.22
4	F	310	PHE	N-CA-C	-5.22	105.48	111.07
5	K	189	ASP	CA-C-N	5.22	132.57	122.07
5	K	189	ASP	C-N-CA	5.22	132.57	122.07
1	M	14	ASP	CB-CA-C	5.22	120.14	109.76
5	K	60(I)	THR	CA-CB-OG1	-5.22	101.77	109.60
5	N	129(B)	LYS	N-CA-C	5.21	118.09	111.69
2	H	60(G)	ASN	OD1-CG-ND2	-5.21	117.39	122.60
2	H	103	ILE	N-CA-C	5.21	115.22	108.35
5	K	166	PRO	CA-C-N	-5.20	111.77	120.30
5	K	166	PRO	C-N-CA	-5.20	111.77	120.30
5	K	47	ILE	CB-CA-C	5.19	120.09	111.37
5	K	169	LYS	CB-CA-C	5.19	119.40	110.79
2	H	60(H)	PHE	CA-CB-CG	-5.18	108.62	113.80
5	K	204(B)	ASN	CB-CA-C	5.18	119.08	110.74
5	N	40	LEU	N-CA-C	-5.17	100.30	108.73
3	E	244	ARG	CD-NE-CZ	-5.17	117.16	124.40
5	K	210	MET	CA-CB-CG	-5.17	103.76	114.10
5	N	181	PHE	N-CA-C	-5.16	101.45	109.24
3	E	214	SER	CB-CA-C	-5.16	104.22	111.65
1	J	1(A)	ASP	CA-C-O	-5.15	113.28	119.15
5	N	211	GLY	N-CA-C	5.14	120.85	110.97
5	K	38	GLN	N-CA-C	5.14	118.42	112.97
4	F	310	PHE	CA-CB-CG	5.14	118.94	113.80
4	G	310	PHE	CA-C-N	5.14	127.43	120.44
4	G	310	PHE	C-N-CA	5.14	127.43	120.44
5	N	175	ARG	CA-C-N	5.14	128.25	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	175	ARG	C-N-CA	5.14	128.25	120.75
5	K	111	PRO	CA-C-O	-5.13	115.41	121.67
5	K	231	VAL	CA-C-O	-5.12	115.74	121.17
5	K	128	THR	O-C-N	5.11	127.98	122.15
4	I	311	LEU	CA-C-N	5.11	127.55	120.29
4	I	311	LEU	C-N-CA	5.11	127.55	120.29
3	E	182	CYS	CB-CA-C	5.11	119.40	109.33
5	K	116	ASP	O-C-N	5.11	128.20	122.22
5	K	209	GLN	CA-C-O	-5.11	115.11	120.58
1	L	14(B)	THR	N-CA-C	5.11	119.60	113.17
5	N	101	ARG	CA-C-O	-5.10	116.35	122.27
5	K	149	THR	N-CA-C	-5.09	99.95	110.80
2	H	62	ASP	CA-CB-CG	5.09	117.69	112.60
3	E	212	ILE	CB-CA-C	-5.09	102.90	110.33
5	N	157	VAL	CA-CB-CG2	5.09	119.05	110.40
5	N	173	ARG	CD-NE-CZ	-5.08	117.28	124.40
3	E	204	PRO	N-CA-C	-5.08	107.41	114.27
5	K	155	LEU	O-C-N	5.08	129.09	122.89
5	N	60(B)	PRO	N-CA-C	5.08	116.90	110.70
1	L	14(K)	ILE	N-CA-C	-5.07	98.80	109.34
5	N	169	LYS	CA-C-O	-5.07	115.18	120.55
3	E	219	GLY	N-CA-C	-5.06	103.47	112.58
5	K	43	GLY	CA-C-O	-5.06	115.13	122.52
2	H	70	LYS	CA-C-O	5.05	127.67	121.72
5	N	123	LEU	CB-CA-C	5.05	115.52	109.31
3	E	241	VAL	CA-C-O	-5.04	115.02	120.47
3	E	151	GLN	OE1-CD-NE2	5.04	127.64	122.60
1	J	14(B)	THR	CB-CA-C	5.04	118.02	109.55
3	E	227	PHE	CA-C-O	-5.03	115.38	120.71
5	K	180	MET	CA-C-O	-5.01	115.59	121.46
2	H	33	LEU	CA-C-O	-5.01	114.88	120.54
5	K	157	VAL	N-CA-C	5.01	115.48	108.17
5	N	225	TYR	CA-CB-CG	-5.01	104.88	113.90
2	H	144	ARG	CA-CB-CG	5.01	124.11	114.10
3	E	234	LEU	CA-C-N	5.01	126.99	120.28
3	E	234	LEU	C-N-CA	5.01	126.99	120.28
1	L	14(K)	ILE	CA-C-O	-5.00	114.53	120.78
2	H	139	THR	CA-CB-OG1	-5.00	102.10	109.60

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	165	ARG	Sidechain
3	E	175	ARG	Sidechain
4	G	318	ARG	Sidechain
2	H	110	ARG	Sidechain
2	H	67	ARG	Sidechain
1	J	15	ARG	Sidechain
5	K	110	ARG	Sidechain
5	K	165	ARG	Sidechain
5	K	175	ARG	Sidechain
5	K	233	ARG	Sidechain
5	K	50	ARG	Sidechain
5	K	77(A)	ARG	Sidechain
5	N	165	ARG	Sidechain
5	N	187	ARG	Sidechain
5	N	206	ARG	Sidechain
5	N	221(A)	ARG	Sidechain
5	N	73	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	J	290	0	276	38	0
1	L	290	0	276	32	0
1	M	290	0	276	47	0
2	H	1235	0	1252	104	0
3	E	860	0	844	89	0
4	F	75	0	69	9	0
4	G	75	0	69	6	0
4	I	75	0	69	9	0
5	K	2094	0	2097	168	0
5	N	2094	0	2097	180	0
6	E	69	0	0	15	0
6	F	10	0	0	0	0
6	G	11	0	0	1	0
6	H	126	0	0	24	0
6	I	9	0	0	6	0
6	J	23	0	0	9	0
6	K	213	0	0	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	31	0	0	6	0
6	M	26	0	0	18	0
6	N	188	0	0	52	0
All	All	8084	0	7325	592	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 40.

All (592) 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)
5:K:60(F):LYS:HB2	6:K:422:HOH:O	1.17	1.28
5:K:176:ILE:HG21	6:K:407:HOH:O	1.27	1.25
1:J:14(G):PHE:HB3	6:J:616:HOH:O	1.30	1.24
5:K:52:VAL:HG22	6:K:432:HOH:O	1.39	1.23
5:N:204:PRO:HB3	6:N:396:HOH:O	1.40	1.21
5:K:169:LYS:HB2	5:K:169:LYS:NZ	1.54	1.16
2:H:62:ASP:HB2	6:H:259:HOH:O	1.42	1.15
3:E:205:ASN:N	6:E:312:HOH:O	1.81	1.11
5:K:233:ARG:HD2	6:K:363:HOH:O	1.48	1.11
5:K:148:TRP:HB2	5:K:150:VAL:HG21	1.35	1.08
5:N:57:HIS:HB3	6:N:427:HOH:O	1.53	1.05
5:N:240:LYS:HG3	5:N:245:LEU:HA	1.12	1.05
5:K:160:LEU:HB3	6:K:308:HOH:O	1.58	1.03
5:K:46:LEU:HD23	6:K:432:HOH:O	1.57	1.03
1:M:14(K):ILE:CG1	6:M:37:HOH:O	2.09	1.01
1:L:15:ARG:CG	2:H:131:HIS:HB3	1.90	1.01
1:L:15:ARG:HG3	2:H:131:HIS:HB3	1.42	1.00
5:N:128:THR:HG22	5:N:129(C):LEU:HD22	1.43	1.00
5:K:235:LYS:HE3	6:K:423:HOH:O	1.60	0.99
1:M:14(K):ILE:HG12	6:M:37:HOH:O	1.63	0.97
4:I:316:GLY:C	6:I:665:HOH:O	2.05	0.97
2:H:144:ARG:NH1	6:H:267:HOH:O	1.98	0.97
6:H:267:HOH:O	3:E:149(E):GLU:HA	1.64	0.95
5:K:41:LEU:HB3	6:K:457:HOH:O	1.66	0.95
5:N:97:LYS:HG2	6:N:334:HOH:O	1.67	0.95
1:J:1(G):PHE:O	6:J:612:HOH:O	1.81	0.95
5:N:119:HIS:CB	6:N:389:HOH:O	2.14	0.94
5:N:149(C):VAL:HA	6:N:399:HOH:O	1.65	0.94
5:N:81:LYS:HD2	5:N:112:ILE:HD11	1.49	0.94
5:K:149(A):THR:HA	5:K:149(D):ALA:O	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:66:VAL:HG21	5:N:85:LEU:HD21	1.52	0.92
5:N:200:VAL:HG12	5:N:209:GLN:HA	1.49	0.92
3:E:165:ARG:H	3:E:165:ARG:HD2	1.32	0.91
3:E:177:THR:HG22	3:E:179:ASN:H	1.33	0.91
5:K:169:LYS:HB2	5:K:169:LYS:HZ3	1.22	0.90
5:N:240:LYS:HD2	5:N:245:LEU:HD22	1.54	0.90
5:K:204(B):ASN:O	5:K:204(B):ASN:ND2	2.05	0.90
5:K:144:ARG:HD3	6:K:433:HOH:O	1.72	0.89
1:M:5:PRO:HD3	6:N:389:HOH:O	1.71	0.89
5:K:244:ARG:O	5:K:245:LEU:HB2	1.71	0.89
1:M:5:PRO:CD	6:N:389:HOH:O	2.19	0.89
1:J:14(A):GLN:HG2	6:J:646:HOH:O	1.69	0.89
5:K:46:LEU:HD22	5:K:48:SER:O	1.72	0.89
2:H:57:HIS:CD2	4:F:317:VAL:HG13	2.08	0.89
3:E:246:GLY:O	3:E:247:SER:HB2	1.71	0.89
2:H:145:ARG:HD2	5:K:149(A):THR:HG21	1.53	0.88
5:K:97:LYS:HD2	6:K:361:HOH:O	1.73	0.88
5:N:147:THR:HG22	5:N:149(B):SER:HB2	1.53	0.88
5:K:148:TRP:HB2	5:K:150:VAL:CG2	2.02	0.88
5:K:164:GLU:HG2	5:K:167:VAL:HG13	1.54	0.88
5:N:195:SER:HB2	4:I:318:ARG:C	1.99	0.87
1:M:3:LEU:HD22	6:N:252:HOH:O	1.74	0.87
4:I:313:GLU:HG3	6:I:675:HOH:O	1.75	0.87
2:H:97(A):GLU:HG3	4:F:308:ACE:H2	1.56	0.87
5:N:240:LYS:HG3	5:N:245:LEU:CA	2.03	0.87
5:N:215:TRP:HB2	6:I:665:HOH:O	1.73	0.86
1:J:1(H):THR:N	1:J:1(C):GLU:OE2	2.06	0.86
5:K:235:LYS:HG3	6:K:423:HOH:O	1.73	0.86
2:H:73:ARG:NH1	3:E:149(C):VAL:HG23	1.90	0.86
5:N:119:HIS:CG	6:N:389:HOH:O	2.27	0.86
3:E:165:ARG:HD2	3:E:165:ARG:N	1.91	0.85
2:H:102:ASP:OD2	6:H:256:HOH:O	1.93	0.85
1:M:1(E):ALA:HB3	6:M:36:HOH:O	1.77	0.85
5:N:240:LYS:CG	5:N:245:LEU:HA	2.05	0.84
1:M:1(H):THR:HB	5:N:235:LYS:HZ2	1.43	0.83
5:N:50:ARG:HD3	6:N:259:HOH:O	1.78	0.83
5:N:66:VAL:CG2	5:N:85:LEU:HD21	2.08	0.82
5:K:176:ILE:CG2	6:K:407:HOH:O	2.00	0.82
5:K:147:THR:HG22	5:K:149(C):VAL:HG11	1.63	0.81
5:K:148:TRP:CG	5:K:149:THR:H	1.97	0.81
1:J:15:ARG:NH1	6:J:696:HOH:O	2.09	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:24:VAL:HB	6:N:388:HOH:O	1.81	0.81
2:H:145:ARG:HD2	5:K:149(A):THR:CG2	2.11	0.81
5:K:169:LYS:HB2	5:K:169:LYS:HZ2	1.46	0.81
5:K:148:TRP:HB3	6:K:317:HOH:O	1.81	0.80
5:N:149(D):ALA:C	5:N:150:VAL:H	1.85	0.80
5:K:38:GLN:OE1	6:K:439:HOH:O	2.00	0.80
2:H:77(A):ARG:HD3	6:H:274:HOH:O	1.82	0.79
5:N:86:ASP:O	5:N:87:LYS:HG3	1.82	0.79
5:K:143:ASN:OD1	6:K:315:HOH:O	2.00	0.78
3:E:165:ARG:CB	6:E:306:HOH:O	2.30	0.78
5:N:81:LYS:CD	5:N:112:ILE:HD11	2.14	0.77
3:E:151:GLN:HB3	6:E:300:HOH:O	1.82	0.77
5:N:119:HIS:HB3	6:N:389:HOH:O	1.76	0.77
2:H:24:VAL:HG23	2:H:117:TYR:HE1	1.49	0.77
5:N:240:LYS:HD3	5:N:245:LEU:HD13	1.67	0.77
5:K:240:LYS:HD2	5:K:247:SER:O	1.84	0.77
5:N:117:TYR:HE1	6:N:388:HOH:O	1.68	0.77
5:K:148:TRP:CD1	5:K:149:THR:H	2.01	0.76
1:L:15:ARG:HG2	2:H:131:HIS:HB3	1.67	0.76
5:K:62:ASP:HB2	6:K:436:HOH:O	1.84	0.76
1:M:14(K):ILE:CD1	6:M:37:HOH:O	2.32	0.76
2:H:99:LEU:HD11	4:F:317:VAL:HG22	1.68	0.76
3:E:165:ARG:HB3	6:E:305:HOH:O	1.86	0.75
2:H:145:ARG:HH21	2:H:149:THR:HG21	1.52	0.75
2:H:73:ARG:HD3	3:E:152:PRO:O	1.86	0.74
5:N:204(B):ASN:O	5:N:206:ARG:N	2.16	0.74
2:H:100:ASP:OD1	3:E:177:THR:HG21	1.86	0.74
1:L:14(K):ILE:C	1:L:14(M):GLY:H	1.95	0.74
5:K:84:MET:HG2	6:K:438:HOH:O	1.86	0.73
3:E:165:ARG:C	6:E:306:HOH:O	2.32	0.73
5:N:149(B):SER:HB2	5:N:150:VAL:HG21	1.70	0.73
1:L:10:LYS:O	1:L:12:VAL:HG23	1.88	0.73
2:H:110:ARG:NE	6:H:185:HOH:O	2.22	0.73
2:H:97(A):GLU:OE2	3:E:175:ARG:HD3	1.89	0.72
2:H:148:TRP:HD1	5:K:149(D):ALA:H	1.37	0.72
1:J:1(F):GLY:HA3	5:K:235:LYS:NZ	2.04	0.72
2:H:148:TRP:HD1	5:K:149(D):ALA:N	1.86	0.72
1:L:14(K):ILE:C	6:L:591:HOH:O	2.32	0.72
5:N:119:HIS:CD2	6:N:389:HOH:O	2.43	0.72
5:N:170:ALA:HA	6:N:431:HOH:O	1.89	0.72
3:E:165:ARG:HB3	6:E:306:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:149(E):GLU:O	3:E:150:VAL:HG12	1.89	0.72
5:K:148:TRP:CG	5:K:149:THR:N	2.55	0.72
5:N:57:HIS:CB	6:N:427:HOH:O	2.25	0.72
5:K:38:GLN:HB2	6:K:458:HOH:O	1.90	0.71
5:K:235:LYS:CG	6:K:423:HOH:O	2.32	0.71
5:K:178:ASP:O	5:K:233:ARG:HD3	1.91	0.71
5:K:164:GLU:CG	5:K:167:VAL:HG13	2.20	0.71
1:M:5:PRO:HG2	5:N:116:ASP:O	1.90	0.71
5:K:205:ASN:N	6:K:431:HOH:O	2.24	0.70
1:L:1(C):GLU:O	1:L:1(B):ALA:HB3	1.91	0.70
5:K:245:LEU:HD12	5:K:247:SER:OXT	1.90	0.70
5:N:244:ARG:O	5:N:245:LEU:HB2	1.91	0.70
5:K:148:TRP:CZ2	6:K:315:HOH:O	2.43	0.70
5:K:208:TYR:CB	5:K:210:MET:HE2	2.21	0.70
5:K:204(B):ASN:HD22	5:K:204(B):ASN:C	1.99	0.70
5:N:60(I):THR:HB	6:N:363:HOH:O	1.93	0.69
6:H:256:HOH:O	3:E:214:SER:OG	2.05	0.69
3:E:204(B):ASN:C	6:E:312:HOH:O	2.20	0.69
3:E:204(B):ASN:ND2	3:E:204(B):ASN:O	2.24	0.69
5:K:143:ASN:ND2	5:K:192:GLU:HG3	2.08	0.69
1:L:10:LYS:HD2	6:L:338:HOH:O	1.91	0.69
3:E:165:ARG:HD3	3:E:166:PRO:HD3	1.75	0.69
3:E:240:LYS:HD3	3:E:247:SER:H	1.56	0.69
5:N:58:CYS:O	6:N:287:HOH:O	2.11	0.69
1:M:14(K):ILE:HD13	6:M:37:HOH:O	1.90	0.68
5:N:203:SER:C	6:N:390:HOH:O	2.37	0.68
1:L:1(C):GLU:O	1:L:1(B):ALA:CB	2.41	0.68
5:K:145:ARG:O	6:K:317:HOH:O	2.10	0.68
2:H:149:THR:OG1	2:H:149(A):THR:N	2.27	0.68
5:N:204(B):ASN:O	5:N:204(B):ASN:ND2	2.27	0.68
4:G:317:VAL:HG13	6:G:589:HOH:O	1.93	0.67
1:M:5:PRO:O	1:M:9:LYS:HB2	1.94	0.67
5:N:169:LYS:NZ	6:N:338:HOH:O	2.28	0.67
5:K:204(B):ASN:C	6:K:431:HOH:O	2.36	0.67
5:N:137:ARG:NH1	5:N:207:TRP:CH2	2.62	0.67
3:E:165:ARG:CD	3:E:166:PRO:HD3	2.25	0.67
5:N:203:SER:O	6:N:390:HOH:O	2.13	0.67
2:H:146:GLU:OE1	3:E:221(A):ARG:NH2	2.28	0.67
5:N:149(B):SER:CB	5:N:150:VAL:HG21	2.25	0.67
5:K:149:THR:O	5:K:149(B):SER:N	2.26	0.66
3:E:245:LEU:N	3:E:245:LEU:HD22	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:22:ALA:HB2	5:K:157:VAL:HG22	1.78	0.66
5:N:173:ARG:NH1	5:N:173:ARG:HG3	2.08	0.66
5:K:33:LEU:HD22	6:K:388:HOH:O	1.94	0.66
5:K:33:LEU:HD13	6:K:388:HOH:O	1.95	0.66
5:N:131:HIS:HD2	5:N:134:PHE:CE2	2.14	0.66
1:J:1(F):GLY:HA3	5:K:235:LYS:HZ2	1.60	0.65
5:K:149(A):THR:O	5:K:149(D):ALA:N	2.29	0.65
3:E:149(C):VAL:HG22	3:E:149(D):ALA:H	1.61	0.65
5:K:148:TRP:CB	5:K:150:VAL:HG21	2.22	0.65
5:N:239:GLN:NE2	5:N:247:SER:HB2	2.11	0.65
1:J:14(M):GLY:HA3	5:K:134:PHE:HE1	1.62	0.65
5:K:74:THR:HA	6:K:337:HOH:O	1.96	0.65
1:J:1(H):THR:HA	6:J:613:HOH:O	1.95	0.65
2:H:75:ARG:NH2	6:H:269:HOH:O	2.27	0.64
2:H:115:SER:O	6:H:260:HOH:O	2.14	0.64
1:J:1(E):ALA:HA	5:K:125:ASP:OD2	1.98	0.64
1:M:3:LEU:CD2	6:N:252:HOH:O	2.38	0.64
5:N:243:ASP:HB3	5:N:244:ARG:HD2	1.80	0.64
2:H:61:VAL:HG22	2:H:85:LEU:HB2	1.80	0.64
5:N:60(D):TRP:NE1	6:N:326:HOH:O	2.19	0.64
5:K:208:TYR:HB2	5:K:210:MET:HE2	1.80	0.64
5:K:105:LEU:HD11	5:K:238:ILE:HG23	1.80	0.63
5:N:149(B):SER:O	5:N:149(C):VAL:HG13	1.99	0.63
5:K:246:GLY:C	6:K:417:HOH:O	2.41	0.63
3:E:165:ARG:H	3:E:165:ARG:CD	1.87	0.62
1:J:1(C):GLU:HG2	1:J:1:CYS:HB3	1.81	0.62
5:K:160:LEU:HD23	6:K:308:HOH:O	1.98	0.62
1:M:5:PRO:HD3	6:M:35:HOH:O	1.98	0.62
5:K:73:ARG:HD3	5:K:152:PRO:O	1.98	0.62
5:K:147:THR:HG23	5:K:149(C):VAL:HG21	1.79	0.62
5:N:57:HIS:CE1	5:N:195:SER:OG	2.52	0.62
3:E:165:ARG:CA	6:E:306:HOH:O	2.47	0.62
5:K:128:THR:HG23	5:K:129(C):LEU:HD22	1.82	0.62
5:K:195:SER:OG	4:G:318:ARG:C	2.42	0.62
5:N:87:LYS:HG2	6:N:433:HOH:O	1.98	0.62
5:K:148:TRP:CZ3	5:K:192:GLU:OE2	2.52	0.62
5:N:240:LYS:O	5:N:240:LYS:HG2	1.99	0.62
5:N:186(A):GLY:N	6:N:318:HOH:O	2.09	0.62
5:K:73:ARG:HB2	5:K:141:TRP:CD1	2.35	0.62
1:J:1(H):THR:HG23	5:K:48:SER:CB	2.30	0.61
3:E:204(B):ASN:C	3:E:204(B):ASN:HD22	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1(B):ALA:C	5:K:206:ARG:HH12	2.08	0.61
5:N:149(A):THR:HB	6:N:435:HOH:O	2.00	0.61
5:N:149(D):ALA:C	5:N:150:VAL:N	2.54	0.61
3:E:177:THR:HG22	3:E:179:ASN:N	2.13	0.61
1:J:14(H):GLU:O	1:J:14(L):GLU:HG3	2.00	0.61
5:N:81:LYS:CG	5:N:112:ILE:HD11	2.31	0.61
3:E:236:LYS:NZ	3:E:239:GLN:OE1	2.32	0.61
5:K:60(F):LYS:HD2	6:K:422:HOH:O	1.95	0.61
2:H:50:ARG:HD3	2:H:111:PRO:HD3	1.82	0.61
2:H:114:LEU:O	2:H:115:SER:HB3	1.99	0.61
1:J:1(H):THR:HG23	5:K:48:SER:OG	2.01	0.60
5:N:165:ARG:NH1	6:N:331:HOH:O	2.34	0.60
5:N:71:HIS:NE2	5:N:154:VAL:CG2	2.64	0.60
5:N:149(C):VAL:O	5:N:151:GLN:NE2	2.35	0.60
1:M:6:LEU:O	6:M:27:HOH:O	2.16	0.60
5:N:147:THR:HG22	5:N:149(B):SER:CB	2.27	0.60
5:K:208:TYR:HB3	5:K:210:MET:HE2	1.83	0.60
2:H:60(D):TRP:HB3	6:H:233:HOH:O	2.00	0.59
2:H:97:LYS:HE3	6:H:151:HOH:O	2.01	0.59
3:E:203:SER:HB3	3:E:204(B):ASN:O	2.02	0.59
1:L:6:LEU:HA	1:L:10:LYS:HD3	1.83	0.59
5:N:60(F):LYS:HD3	6:N:287:HOH:O	2.02	0.59
1:L:15:ARG:HG3	2:H:131:HIS:CB	2.26	0.59
5:N:114:LEU:O	5:N:115:SER:OG	2.20	0.59
5:K:62:ASP:CB	6:K:436:HOH:O	2.45	0.59
5:K:78:LYS:HE2	6:K:399:HOH:O	2.01	0.59
5:N:239:GLN:NE2	5:N:247:SER:OXT	2.35	0.59
4:I:317:VAL:N	6:I:665:HOH:O	2.31	0.59
1:L:14(C):GLU:OE2	3:E:202:LYS:NZ	2.28	0.59
1:L:14(J):TYR:O	1:L:14(K):ILE:HB	2.01	0.59
2:H:149(A):THR:OXT	3:E:150:VAL:HG11	2.02	0.59
1:M:14(K):ILE:HG23	6:M:37:HOH:O	2.02	0.59
1:L:14(E):GLU:OE2	3:E:186(D):LYS:NZ	2.36	0.58
5:K:87:LYS:HD2	5:K:89:TYR:CZ	2.37	0.58
3:E:149(B):SER:O	3:E:149(C):VAL:HB	2.02	0.58
5:K:247:SER:HB2	6:K:417:HOH:O	2.03	0.58
2:H:81:LYS:HE3	6:H:239:HOH:O	2.03	0.58
3:E:177:THR:HG22	3:E:179:ASN:HB2	1.84	0.58
5:K:36:LYS:HD3	6:K:438:HOH:O	2.03	0.58
5:K:148:TRP:HZ3	5:K:192:GLU:OE2	1.85	0.58
6:M:38:HOH:O	5:N:129(C):LEU:HG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:16:ILE:N	5:N:194:ASP:OD2	2.37	0.58
2:H:145:ARG:HG2	3:E:150:VAL:HG23	1.85	0.58
5:N:165:ARG:HB3	5:N:166:PRO:HD3	1.85	0.58
5:N:46:LEU:HD22	5:N:48:SER:O	2.04	0.58
1:J:1(C):GLU:CG	1:J:1:CYS:HB3	2.35	0.57
5:N:239:GLN:CD	5:N:247:SER:HB2	2.29	0.57
5:N:143:ASN:OD1	5:N:192:GLU:HG3	2.05	0.57
2:H:73:ARG:HH12	3:E:149(C):VAL:HA	1.69	0.57
2:H:32:MET:HG3	2:H:40:LEU:CD2	2.34	0.57
3:E:177:THR:HB	3:E:180:MET:HE3	1.87	0.57
5:N:147:THR:O	5:N:148:TRP:CD1	2.57	0.57
5:N:147:THR:CG2	5:N:150:VAL:HG11	2.34	0.56
3:E:149(C):VAL:HG13	3:E:149(D):ALA:N	2.20	0.56
1:J:1(F):GLY:O	1:J:1(E):ALA:HB2	2.04	0.56
1:J:1(C):GLU:C	1:J:1(A):ASP:H	2.14	0.56
5:N:24:VAL:CB	6:N:388:HOH:O	2.48	0.56
5:N:243:ASP:C	5:N:244:ARG:HD2	2.30	0.56
5:K:129(C):LEU:HD23	5:K:210:MET:HE3	1.88	0.56
2:H:36(A):SER:HA	2:H:37:PRO:C	2.31	0.56
3:E:149(D):ALA:O	3:E:151:GLN:HG2	2.05	0.56
1:J:15:ARG:HA	6:J:680:HOH:O	2.04	0.56
5:K:60(I):THR:O	5:K:63:ASP:HB2	2.06	0.56
5:N:147:THR:HA	5:N:149(B):SER:OG	2.05	0.56
2:H:32:MET:HG3	2:H:40:LEU:HD23	1.87	0.56
1:M:5:PRO:CD	6:M:35:HOH:O	2.54	0.56
2:H:146:GLU:HB3	5:K:149(B):SER:HB2	1.88	0.56
5:N:136:GLY:HA3	5:N:199:PHE:CZ	2.39	0.56
2:H:29:TRP:CD2	2:H:121:VAL:HB	2.41	0.56
1:J:1(C):GLU:O	1:J:1(B):ALA:HB3	2.05	0.56
1:M:14(K):ILE:CG2	6:M:37:HOH:O	2.54	0.56
5:K:113:GLU:HG3	6:K:446:HOH:O	2.05	0.56
1:L:14(K):ILE:O	6:L:591:HOH:O	2.18	0.55
5:K:34:PHE:HE1	6:K:458:HOH:O	1.89	0.55
1:J:14(M):GLY:HA3	5:K:134:PHE:CE1	2.41	0.55
3:E:204(B):ASN:CA	6:E:312:HOH:O	2.53	0.55
5:K:52:VAL:CG2	6:K:432:HOH:O	2.17	0.55
1:L:14(A):GLN:HB3	6:L:511:HOH:O	2.06	0.55
2:H:24:VAL:HG23	2:H:117:TYR:CE1	2.35	0.55
2:H:74:THR:HG22	2:H:75:ARG:N	2.21	0.55
5:K:239:GLN:HG3	6:K:417:HOH:O	2.05	0.55
1:L:1(D):GLY:HA2	6:L:158:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:3:LEU:HD21	5:N:206:ARG:HG2	1.89	0.55
5:N:171:SER:O	5:N:224:LYS:NZ	2.37	0.55
4:I:316:GLY:O	6:I:665:HOH:O	2.18	0.55
2:H:97(A):GLU:CD	3:E:175:ARG:HH11	2.15	0.54
3:E:165:ARG:N	3:E:165:ARG:CD	2.55	0.54
5:K:149(A):THR:CA	5:K:149(D):ALA:O	2.50	0.54
2:H:66:VAL:HG12	2:H:83:SER:OG	2.07	0.54
4:I:310:PHE:HZ	6:I:665:HOH:O	1.90	0.54
3:E:173:ARG:HB2	4:F:313:GLU:OE1	2.07	0.54
1:M:14(E):GLU:HB2	6:M:33:HOH:O	2.06	0.54
5:N:81:LYS:HG3	5:N:112:ILE:HD11	1.90	0.54
1:L:1:CYS:O	3:E:206:ARG:HD3	2.07	0.54
2:H:139:THR:HA	3:E:156:GLN:O	2.08	0.54
5:K:148:TRP:CD1	5:K:150:VAL:CG2	2.91	0.54
5:K:17:VAL:O	5:K:188:GLY:HA2	2.08	0.54
5:N:221(A):ARG:NH2	6:N:429:HOH:O	2.41	0.54
5:N:29:TRP:O	5:N:45:SER:HA	2.08	0.54
5:N:240:LYS:CB	5:N:246:GLY:H	2.21	0.54
1:J:1(F):GLY:HA2	5:K:123:LEU:HB2	1.88	0.54
5:K:211:GLY:HA2	5:K:229:THR:O	2.08	0.54
5:K:22:ALA:O	5:K:71:HIS:HE1	1.91	0.54
2:H:60(B):PRO:HB2	2:H:60(C):PRO:HD3	1.90	0.53
2:H:97(A):GLU:HG3	4:F:308:ACE:CH3	2.33	0.53
5:K:127:GLN:O	5:K:129(B):LYS:HD3	2.08	0.53
1:M:4:ARG:O	1:M:5:PRO:C	2.50	0.53
2:H:97(A):GLU:O	4:F:310:PHE:HB2	2.07	0.53
5:N:204:PRO:HA	6:N:390:HOH:O	2.07	0.53
3:E:221(A):ARG:HD3	6:E:311:HOH:O	2.09	0.53
1:J:1(B):ALA:HA	5:K:206:ARG:HH22	1.73	0.53
1:L:1(E):ALA:HB2	3:E:206:ARG:CZ	2.39	0.53
6:H:256:HOH:O	3:E:214:SER:CB	2.54	0.53
5:N:27:SER:OG	5:N:29:TRP:NE1	2.42	0.53
5:N:128:THR:O	5:N:129(C):LEU:HB2	2.09	0.53
3:E:177:THR:CG2	3:E:179:ASN:HB2	2.39	0.53
1:J:1(D):GLY:C	1:J:1(B):ALA:H	2.15	0.53
5:N:125:ASP:OD1	5:N:128:THR:OG1	2.27	0.52
5:N:127:GLN:O	5:N:129(B):LYS:HD2	2.09	0.52
1:M:6:LEU:HD11	5:N:116:ASP:HB3	1.90	0.52
5:N:236:LYS:HE3	5:N:247:SER:OG	2.10	0.52
5:N:203:SER:HG	5:N:204(A):TYR:HD2	1.57	0.52
3:E:214:SER:HB3	3:E:215:TRP:HD1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:113:GLU:HG2	6:H:239:HOH:O	2.09	0.52
1:J:1(H):THR:HG23	5:K:48:SER:HB3	1.92	0.52
1:J:12:VAL:HG13	6:J:517:HOH:O	2.10	0.52
2:H:17:VAL:O	3:E:188:GLY:HA2	2.09	0.52
1:M:8:GLU:HG2	6:N:252:HOH:O	2.09	0.52
5:N:79:VAL:HG12	5:N:117:TYR:CD2	2.43	0.52
5:N:117:TYR:CE1	6:N:388:HOH:O	2.51	0.52
5:N:81:LYS:HD2	5:N:112:ILE:CD1	2.30	0.52
2:H:149(A):THR:O	6:H:197:HOH:O	2.19	0.51
1:M:14(C):GLU:OE2	5:N:202:LYS:NZ	2.39	0.51
5:N:66:VAL:HG12	5:N:68:ILE:HD11	1.92	0.51
5:K:60(F):LYS:HG3	5:K:60(H):PHE:CE2	2.45	0.51
5:K:148:TRP:CB	6:K:317:HOH:O	2.48	0.51
3:E:236:LYS:N	3:E:236:LYS:HD2	2.20	0.51
5:N:152:PRO:HG3	6:N:422:HOH:O	2.09	0.51
2:H:74:THR:HG21	3:E:149(B):SER:HB2	1.92	0.51
5:N:24:VAL:CG2	6:N:388:HOH:O	2.59	0.51
5:K:38:GLN:HB2	6:K:459:HOH:O	2.11	0.51
1:J:1(D):GLY:HA2	1:J:1:CYS:SG	2.51	0.51
5:K:86:ASP:HB3	5:K:107:LYS:HG3	1.93	0.51
5:K:97:LYS:HE2	6:K:257:HOH:O	2.10	0.51
5:N:93:ARG:HG2	5:N:93:ARG:HH11	1.76	0.51
5:N:204(B):ASN:HD22	5:N:206:ARG:HG3	1.76	0.51
5:N:237:TRP:O	5:N:241:VAL:HG13	2.12	0.50
5:K:60(F):LYS:CB	6:K:422:HOH:O	2.02	0.50
5:K:185:LYS:HB2	5:K:186(B):GLU:OE1	2.11	0.50
3:E:149(D):ALA:HB3	3:E:151:GLN:HE21	1.76	0.50
5:K:40:LEU:C	5:K:40:LEU:HD23	2.37	0.50
5:K:235:LYS:CD	6:K:423:HOH:O	2.59	0.50
5:N:240:LYS:HB2	5:N:246:GLY:H	1.77	0.50
2:H:50:ARG:CD	6:H:172:HOH:O	2.60	0.50
5:K:160:LEU:CG	6:K:308:HOH:O	2.58	0.50
1:M:1(E):ALA:O	1:M:1(D):GLY:C	2.55	0.50
5:N:186(A):GLY:CA	6:N:318:HOH:O	2.55	0.50
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.74	0.50
2:H:74:THR:HG22	2:H:75:ARG:H	1.77	0.50
3:E:221(A):ARG:CD	6:E:311:HOH:O	2.59	0.50
5:K:34:PHE:CE1	5:K:38:GLN:O	2.65	0.50
3:E:176:ILE:HD11	3:E:215:TRP:HZ2	1.77	0.49
3:E:239:GLN:NE2	6:E:294:HOH:O	1.99	0.49
5:K:128:THR:HG22	5:K:210:MET:HE1	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:163:VAL:CG1	5:K:167:VAL:HG22	2.42	0.49
5:N:239:GLN:HB3	5:N:247:SER:HA	1.94	0.49
5:K:127:GLN:HG3	5:K:129(B):LYS:CE	2.42	0.49
5:N:239:GLN:NE2	5:N:247:SER:CA	2.75	0.49
5:N:197:GLY:HA3	6:N:278:HOH:O	2.11	0.49
3:E:176:ILE:HG13	3:E:227:PHE:CE2	2.46	0.49
1:M:1(H):THR:CB	5:N:235:LYS:HZ2	2.22	0.49
5:N:91:HIS:ND1	5:N:92:PRO:HD2	2.27	0.49
1:J:1(H):THR:O	1:J:1(G):PHE:CD1	2.66	0.49
5:N:204(B):ASN:O	5:N:206:ARG:HG3	2.12	0.49
5:N:144:ARG:NH2	5:N:152:PRO:HA	2.27	0.49
2:H:149(A):THR:OXT	3:E:150:VAL:CG1	2.59	0.49
5:N:57:HIS:HE1	5:N:195:SER:OG	1.94	0.49
5:N:128:THR:CG2	5:N:129(C):LEU:HD22	2.30	0.49
6:H:273:HOH:O	3:E:152:PRO:HG3	2.12	0.49
5:K:45:SER:O	5:K:52:VAL:HA	2.13	0.48
5:N:59:LEU:HD11	5:N:106:LEU:HD11	1.93	0.48
1:L:14(J):TYR:O	1:L:14(K):ILE:CB	2.61	0.48
5:K:127:GLN:CD	6:K:378:HOH:O	2.56	0.48
1:L:1(E):ALA:HB1	3:E:206:ARG:NH1	2.28	0.48
1:J:1(H):THR:CA	6:J:613:HOH:O	2.58	0.48
2:H:53:LEU:HD11	2:H:103:ILE:HD11	1.95	0.48
5:K:60(B):PRO:HB2	5:K:60(C):PRO:HD3	1.94	0.48
3:E:201:MET:SD	3:E:210:MET:HG3	2.53	0.48
5:K:195:SER:HG	4:G:318:ARG:C	2.21	0.48
5:N:186(A):GLY:HA3	6:N:318:HOH:O	2.13	0.48
5:N:185:LYS:HG3	5:N:186(B):GLU:OE1	2.14	0.48
1:L:1(C):GLU:OE1	2:H:120:PRO:HG2	2.14	0.48
3:E:215:TRP:HB2	4:F:316:GLY:O	2.14	0.48
5:K:143:ASN:ND2	6:K:317:HOH:O	2.46	0.48
5:N:86:ASP:HB2	5:N:109:LYS:HA	1.95	0.48
5:N:50:ARG:HE	5:N:111:PRO:HG3	1.79	0.47
1:L:15:ARG:CZ	2:H:132:ALA:HB3	2.44	0.47
3:E:244:ARG:C	3:E:245:LEU:HD22	2.39	0.47
2:H:148:TRP:CD1	5:K:149(D):ALA:N	2.76	0.47
5:K:95:ASN:O	5:K:99:LEU:HA	2.14	0.47
5:K:149(A):THR:C	5:K:149(C):VAL:N	2.67	0.47
2:H:73:ARG:HB2	2:H:141:TRP:CD1	2.50	0.47
2:H:31:VAL:HG22	2:H:68:ILE:HG12	1.96	0.47
2:H:32:MET:SD	2:H:67:ARG:HD3	2.54	0.47
2:H:68:ILE:HA	6:H:261:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:146:GLU:HG3	3:E:220:CYS:H	1.78	0.47
5:N:53:LEU:HD11	5:N:103:ILE:HD11	1.97	0.47
2:H:96:TRP:HA	2:H:99:LEU:HD23	1.96	0.47
5:K:148:TRP:HE1	5:K:151:GLN:HE21	1.63	0.47
5:N:35:ARG:O	5:N:38:GLN:HA	2.15	0.47
5:N:151:GLN:HB3	6:N:282:HOH:O	2.15	0.47
5:N:240:LYS:CG	5:N:240:LYS:O	2.61	0.47
5:N:139:THR:HG22	5:N:156:GLN:O	2.14	0.47
5:N:204:PRO:CB	6:N:396:HOH:O	2.22	0.47
5:N:204(B):ASN:HD22	5:N:206:ARG:CG	2.28	0.47
5:N:131:HIS:HD2	5:N:134:PHE:HE2	1.60	0.47
5:N:221(A):ARG:NH2	6:N:329:HOH:O	2.47	0.47
3:E:185:LYS:HG3	3:E:225:TYR:OH	2.15	0.47
1:J:1(F):GLY:O	1:J:1(E):ALA:CB	2.63	0.47
5:K:149:THR:O	5:K:149:THR:CG2	2.63	0.47
1:M:14(J):TYR:OH	6:M:25:HOH:O	2.18	0.47
5:N:221(A):ARG:NH1	6:N:429:HOH:O	2.48	0.47
2:H:143:ASN:HD22	3:E:192:GLU:CD	2.21	0.46
5:K:34:PHE:HB3	5:K:65:LEU:HD12	1.97	0.46
5:K:165:ARG:N	5:K:166:PRO:CD	2.77	0.46
5:N:76:TYR:HE1	5:N:82:ILE:HD11	1.80	0.46
5:N:95:ASN:O	5:N:99:LEU:HA	2.14	0.46
1:L:1(E):ALA:CB	3:E:206:ARG:CZ	2.93	0.46
5:K:119:HIS:HA	5:K:120:PRO:HD3	1.77	0.46
5:K:247:SER:HB3	6:K:275:HOH:O	2.16	0.46
2:H:81:LYS:HA	2:H:81:LYS:HD3	1.80	0.46
2:H:146:GLU:OE2	5:K:149:THR:HG22	2.14	0.46
3:E:229:THR:CG2	3:E:234:LEU:HD12	2.46	0.46
5:K:60(F):LYS:NZ	6:K:457:HOH:O	2.48	0.46
5:K:145:ARG:HE	5:K:149(C):VAL:HG11	1.80	0.46
5:N:148:TRP:CD2	6:N:414:HOH:O	2.68	0.46
5:N:203:SER:OG	5:N:204(A):TYR:HD2	1.98	0.46
5:N:239:GLN:NE2	5:N:247:SER:HA	2.30	0.46
2:H:70:LYS:HE3	2:H:72:SER:O	2.16	0.46
3:E:164:GLU:HB2	3:E:165:ARG:HD2	1.97	0.46
5:K:127:GLN:HG2	6:K:378:HOH:O	2.16	0.46
2:H:59:LEU:HD11	2:H:106:LEU:HD11	1.98	0.46
5:N:240:LYS:CD	5:N:245:LEU:HD13	2.43	0.46
1:L:15:ARG:HG2	2:H:132:ALA:O	2.16	0.45
1:J:1(F):GLY:HA2	6:J:612:HOH:O	2.15	0.45
5:N:178:ASP:HB3	5:N:233:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:236:LYS:HG3	5:N:247:SER:HB3	1.98	0.45
5:K:148:TRP:CD1	5:K:150:VAL:HG22	2.51	0.45
1:M:1(G):PHE:HD2	1:M:1(E):ALA:HB2	1.80	0.45
5:N:24:VAL:HG23	6:N:388:HOH:O	2.15	0.45
5:N:149(A):THR:O	6:N:435:HOH:O	2.20	0.45
2:H:79:VAL:HG21	6:H:247:HOH:O	2.15	0.45
2:H:148:TRP:CD1	5:K:149(C):VAL:HA	2.51	0.45
3:E:246:GLY:O	3:E:247:SER:CB	2.51	0.45
5:K:128:THR:CG2	5:K:129(C):LEU:HD22	2.47	0.45
5:K:161:PRO:HG2	5:K:184:GLY:O	2.15	0.45
5:N:73:ARG:NH1	5:N:152:PRO:O	2.43	0.45
5:K:169:LYS:HE3	6:K:250:HOH:O	2.17	0.45
1:M:1(H):THR:HG22	1:M:1(G):PHE:O	2.16	0.45
5:N:17:VAL:HG23	5:N:191:CYS:HB2	1.99	0.45
5:N:71:HIS:CD2	5:N:154:VAL:HG23	2.52	0.45
5:N:139:THR:HA	5:N:156:GLN:O	2.16	0.45
2:H:128:THR:HG23	2:H:129(C):LEU:HD22	1.99	0.45
5:K:148:TRP:CB	5:K:150:VAL:CG2	2.87	0.45
1:M:3:LEU:CD2	5:N:206:ARG:HG2	2.46	0.45
1:M:4:ARG:HA	1:M:5:PRO:HD2	1.80	0.45
5:N:60(B):PRO:O	5:N:60(D):TRP:N	2.49	0.45
3:E:239:GLN:HE21	3:E:239:GLN:HB3	1.40	0.45
5:K:203:SER:HA	5:K:204:PRO:HD3	1.76	0.45
5:K:240:LYS:HD2	5:K:247:SER:C	2.42	0.45
1:M:1(C):GLU:CB	1:M:1:CYS:HB3	2.47	0.45
5:N:165:ARG:NE	6:N:375:HOH:O	2.43	0.45
5:K:146:GLU:OE2	5:K:221(A):ARG:HD3	2.17	0.45
2:H:68:ILE:HG22	2:H:118:ILE:HG12	1.97	0.45
1:J:1(C):GLU:C	1:J:1(A):ASP:N	2.73	0.45
2:H:57:HIS:NE2	4:F:317:VAL:HG13	2.29	0.45
3:E:244:ARG:NE	6:E:307:HOH:O	2.25	0.45
2:H:147:THR:O	2:H:147:THR:HG22	2.16	0.45
2:H:66:VAL:HG11	2:H:108:LEU:HD21	1.99	0.44
1:J:14(M):GLY:O	1:J:15:ARG:CB	2.65	0.44
1:M:8:GLU:HB3	6:N:252:HOH:O	2.17	0.44
1:L:1:CYS:C	2:H:122:CYS:SG	3.00	0.44
5:N:239:GLN:NE2	5:N:247:SER:CB	2.80	0.44
1:J:1(F):GLY:CA	5:K:123:LEU:HB2	2.46	0.44
3:E:149(C):VAL:O	3:E:149(D):ALA:HB2	2.17	0.44
3:E:171:SER:O	3:E:224:LYS:NZ	2.45	0.44
5:N:71:HIS:CD2	5:N:154:VAL:CG2	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:98:ASN:O	2:H:99:LEU:HB2	2.18	0.44
5:K:204(B):ASN:O	5:K:206:ARG:N	2.43	0.44
5:N:91:HIS:CG	5:N:92:PRO:HD2	2.52	0.44
2:H:61:VAL:HG23	2:H:88:ILE:HG13	1.99	0.44
1:J:1:CYS:C	5:K:122:CYS:SG	3.01	0.44
1:M:1(H):THR:N	5:N:239:GLN:NE2	2.66	0.44
3:E:245:LEU:N	3:E:245:LEU:CD2	2.80	0.44
5:K:89:TYR:O	5:K:104:ALA:HA	2.18	0.44
4:G:311:LEU:HD12	4:G:311:LEU:HA	1.66	0.44
1:M:1(G):PHE:HB3	5:N:125:ASP:HB3	1.98	0.44
2:H:143:ASN:ND2	3:E:192:GLU:CG	2.81	0.44
2:H:98:ASN:OD1	2:H:98:ASN:N	2.50	0.43
1:M:14(F):LEU:HD21	5:N:159:ASN:OD1	2.18	0.43
5:N:173:ARG:NH1	5:N:173:ARG:CG	2.72	0.43
2:H:87:LYS:HD2	2:H:88:ILE:H	1.82	0.43
2:H:146:GLU:CD	5:K:149(B):SER:HB2	2.43	0.43
5:K:73:ARG:NH2	6:K:336:HOH:O	2.51	0.43
5:N:223:GLY:O	6:N:416:HOH:O	2.21	0.43
2:H:50:ARG:HD3	6:H:172:HOH:O	2.19	0.43
2:H:74:THR:CG2	2:H:75:ARG:N	2.81	0.43
1:J:1(E):ALA:O	5:K:208:TYR:OH	2.26	0.43
1:M:1(G):PHE:N	6:M:36:HOH:O	2.50	0.43
1:M:3:LEU:HD11	5:N:206:ARG:HH21	1.83	0.43
5:N:77(A):ARG:HH21	5:N:78:LYS:HD2	1.83	0.43
5:K:22:ALA:HB2	5:K:157:VAL:CG2	2.46	0.43
2:H:84:MET:SD	6:H:234:HOH:O	2.62	0.43
2:H:34:PHE:HE1	6:H:241:HOH:O	2.01	0.43
5:N:66:VAL:HG23	5:N:85:LEU:HD21	1.95	0.43
5:K:224:LYS:HA	5:K:224:LYS:HD3	1.85	0.43
5:N:94:TYR:CE1	6:N:427:HOH:O	2.72	0.43
1:J:14(G):PHE:CE1	5:K:202:LYS:HD3	2.54	0.43
5:K:50:ARG:HE	5:K:111:PRO:HB3	1.83	0.43
5:K:148:TRP:CD1	5:K:149:THR:N	2.80	0.43
5:N:204(B):ASN:ND2	5:N:206:ARG:HD2	2.34	0.43
1:L:1(E):ALA:CB	3:E:206:ARG:NH1	2.82	0.43
2:H:146:GLU:OE2	5:K:149:THR:CG2	2.67	0.43
1:M:14(I):SER:HB3	6:M:39:HOH:O	2.19	0.43
2:H:101:ARG:NH1	6:H:153:HOH:O	2.33	0.42
2:H:128:THR:CG2	2:H:129(C):LEU:HD22	2.49	0.42
5:K:169:LYS:NZ	6:K:407:HOH:O	2.51	0.42
1:M:1(C):GLU:O	1:M:1(A):ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:236:LYS:HB3	6:E:313:HOH:O	2.19	0.42
3:E:244:ARG:HA	3:E:244:ARG:HD3	1.48	0.42
5:N:194:ASP:O	5:N:195:SER:C	2.62	0.42
5:N:195:SER:CB	4:I:318:ARG:C	2.81	0.42
3:E:149(C):VAL:HG22	3:E:151:GLN:O	2.20	0.42
3:E:214:SER:HB3	3:E:215:TRP:CD1	2.53	0.42
1:M:5:PRO:CG	6:M:35:HOH:O	2.67	0.42
5:N:35:ARG:HD2	5:N:39:GLU:OE2	2.20	0.42
3:E:149(C):VAL:HG13	3:E:149(D):ALA:H	1.82	0.42
5:N:212:ILE:O	5:N:228:TYR:HA	2.20	0.42
1:L:14(K):ILE:C	1:L:14(M):GLY:N	2.67	0.42
2:H:32:MET:CG	2:H:40:LEU:HD23	2.48	0.42
5:N:138:VAL:CG2	5:N:199:PHE:HD2	2.32	0.42
5:K:73:ARG:HD2	6:K:434:HOH:O	2.19	0.42
5:K:101:ARG:HH11	5:K:101:ARG:HD2	1.49	0.42
1:J:14(B):THR:HB	5:K:159:ASN:HD21	1.85	0.42
5:K:98:ASN:O	5:K:180:MET:HE1	2.19	0.42
5:K:165:ARG:HB3	5:K:166:PRO:HD3	2.02	0.42
4:I:311:LEU:HD12	4:I:311:LEU:HA	1.74	0.42
2:H:114:LEU:HD12	2:H:118:ILE:HG22	2.02	0.42
3:E:165:ARG:NH1	6:E:290:HOH:O	2.53	0.42
1:M:1(H):THR:HG22	1:M:1(G):PHE:N	2.34	0.42
2:H:31:VAL:CG1	2:H:66:VAL:HG22	2.50	0.42
5:K:57:HIS:CD2	4:G:317:VAL:HB	2.54	0.42
5:N:66:VAL:HG12	5:N:68:ILE:CD1	2.49	0.42
2:H:63:ASP:C	2:H:64:LEU:HG	2.45	0.41
5:N:217:GLU:HB3	6:N:336:HOH:O	2.20	0.41
5:K:189:ASP:OD2	4:G:318:ARG:NH2	2.52	0.41
1:M:1(C):GLU:HB3	1:M:1:CYS:HB3	2.02	0.41
1:L:4:ARG:HA	1:L:5:PRO:HD3	1.91	0.41
2:H:50:ARG:HE	2:H:50:ARG:HB2	1.20	0.41
5:K:34:PHE:HE1	5:K:38:GLN:O	2.02	0.41
5:K:79:VAL:HG11	6:K:351:HOH:O	2.20	0.41
5:N:16:ILE:CD1	5:N:138:VAL:HG12	2.50	0.41
5:N:129(C):LEU:O	5:N:134:PHE:HD2	2.03	0.41
5:N:71:HIS:CE1	5:N:154:VAL:HG22	2.56	0.41
1:L:1(F):GLY:H	2:H:125:ASP:CG	2.29	0.41
2:H:86:ASP:HB3	2:H:107:LYS:HG3	2.01	0.41
5:K:233:ARG:HE	5:K:233:ARG:HB3	1.29	0.41
1:M:1(F):GLY:HA2	6:M:31:HOH:O	2.21	0.41
1:L:1(H):THR:O	2:H:125:ASP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:195:SER:HB2	4:F:318:ARG:C	2.45	0.41
5:N:173:ARG:CG	5:N:173:ARG:HH11	2.33	0.41
5:N:240:LYS:CD	5:N:245:LEU:HD22	2.36	0.41
2:H:16:ILE:O	2:H:144:ARG:HA	2.21	0.41
5:K:32:MET:HE1	5:K:70:LYS:CE	2.50	0.41
5:N:131:HIS:CD2	5:N:134:PHE:CE2	3.01	0.41
1:L:14(A):GLN:CB	6:L:511:HOH:O	2.66	0.41
2:H:130:LEU:HA	3:E:162:LEU:HD21	2.02	0.41
6:H:267:HOH:O	3:E:149(E):GLU:CA	2.41	0.41
5:K:143:ASN:CG	6:K:315:HOH:O	2.59	0.41
1:M:1(H):THR:OG1	5:N:239:GLN:NE2	2.54	0.41
5:N:76:TYR:CE2	5:N:77(A):ARG:HG2	2.55	0.41
5:N:195:SER:HB2	4:I:318:ARG:O	2.19	0.41
5:N:240:LYS:HD2	5:N:245:LEU:CD2	2.36	0.41
5:K:75:ARG:NH1	5:K:75:ARG:HG3	2.35	0.40
5:K:108:LEU:HD13	5:K:112:ILE:CG1	2.51	0.40
5:N:60(A):TYR:OH	6:N:327:HOH:O	2.18	0.40
5:N:137:ARG:NH1	5:N:207:TRP:HH2	2.13	0.40
2:H:134:PHE:N	2:H:134:PHE:CD1	2.88	0.40
5:K:81:LYS:HG2	5:K:118:ILE:CD1	2.51	0.40
5:K:91:HIS:CE1	5:K:93:ARG:HB2	2.56	0.40
1:M:1(H):THR:O	5:N:235:LYS:CE	2.68	0.40
1:M:1:CYS:C	5:N:122:CYS:SG	3.05	0.40
5:N:60(B):PRO:O	5:N:60(C):PRO:C	2.63	0.40
5:N:201:MET:SD	5:N:210:MET:HG3	2.61	0.40
5:N:57:HIS:CA	6:N:427:HOH:O	2.62	0.40
1:M:5:PRO:HG3	6:M:35:HOH:O	2.21	0.40
5:N:93:ARG:HH11	5:N:93:ARG:CG	2.33	0.40
5:N:192:GLU:H	5:N:192:GLU:HG2	1.75	0.40

There are no symmetry-related clashes.

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	J	34/49 (69%)	28 (82%)	5 (15%)	1 (3%)	3	2
1	L	34/49 (69%)	27 (79%)	4 (12%)	3 (9%)	0	0
1	M	34/49 (69%)	26 (76%)	6 (18%)	2 (6%)	1	0
2	H	148/150 (99%)	135 (91%)	13 (9%)	0	100	100
3	E	107/109 (98%)	97 (91%)	7 (6%)	3 (3%)	4	2
4	F	9/11 (82%)	8 (89%)	0	1 (11%)	0	0
4	G	9/11 (82%)	9 (100%)	0	0	100	100
4	I	9/11 (82%)	8 (89%)	1 (11%)	0	100	100
5	K	257/259 (99%)	235 (91%)	19 (7%)	3 (1%)	10	12
5	N	257/259 (99%)	229 (89%)	24 (9%)	4 (2%)	7	7
All	All	898/957 (94%)	802 (89%)	79 (9%)	17 (2%)	6	5

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(B)	ALA
1	L	14(K)	ILE
3	E	149(C)	VAL
3	E	150	VAL
4	F	309	ASP
1	J	1(E)	ALA
5	K	149(A)	THR
5	K	205	ASN
5	K	245	LEU
5	N	205	ASN
5	N	245	LEU
3	E	149(D)	ALA
1	M	1(B)	ALA
5	N	149(A)	THR
5	N	149(C)	VAL
1	L	14(J)	TYR
1	M	5	PRO

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	J	30/43 (70%)	26 (87%)	4 (13%)	4	4
1	L	30/43 (70%)	30 (100%)	0	100	100
1	M	30/43 (70%)	30 (100%)	0	100	100
2	H	134/134 (100%)	115 (86%)	19 (14%)	3	3
3	E	92/92 (100%)	80 (87%)	12 (13%)	4	4
4	F	6/6 (100%)	4 (67%)	2 (33%)	0	0
4	G	6/6 (100%)	5 (83%)	1 (17%)	2	2
4	I	6/6 (100%)	4 (67%)	2 (33%)	0	0
5	K	226/226 (100%)	192 (85%)	34 (15%)	3	3
5	N	226/226 (100%)	194 (86%)	32 (14%)	3	3
All	All	786/825 (95%)	680 (86%)	106 (14%)	4	4

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	24	VAL
2	H	33	LEU
2	H	50	ARG
2	H	61	VAL
2	H	64	LEU
2	H	66	VAL
2	H	74	THR
2	H	97	LYS
2	H	97(A)	GLU
2	H	99	LEU
2	H	106	LEU
2	H	110	ARG
2	H	112	ILE
2	H	114	LEU
2	H	126	LYS
2	H	147	THR
2	H	148	TRP
2	H	149	THR
2	H	149(A)	THR
3	E	157	VAL
3	E	164	GLU
3	E	165	ARG
3	E	174	ILE

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Mol	Chain	Res	Type
3	E	176	ILE
3	E	185	LYS
3	E	192	GLU
3	E	195	SER
3	E	214	SER
3	E	236	LYS
3	E	239	GLN
3	E	241	VAL
4	F	309	ASP
4	F	317	VAL
1	J	6	LEU
1	J	10	LYS
1	J	11	GLN
1	J	15	ARG
5	K	27	SER
5	K	34	PHE
5	K	38	GLN
5	K	40	LEU
5	K	46	LEU
5	K	61	VAL
5	K	63	ASP
5	K	64	LEU
5	K	65	LEU
5	K	66	VAL
5	K	78	LYS
5	K	79	VAL
5	K	110	ARG
5	K	129(B)	LYS
5	K	129(C)	LEU
5	K	130	LEU
5	K	147	THR
5	K	148	TRP
5	K	149	THR
5	K	149(A)	THR
5	K	149(B)	SER
5	K	149(C)	VAL
5	K	149(E)	GLU
5	K	153	SER
5	K	154	VAL
5	K	157	VAL
5	K	160	LEU
5	K	164	GLU

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Mol	Chain	Res	Type
5	K	167	VAL
5	K	169	LYS
5	K	185	LYS
5	K	192	GLU
5	K	241	VAL
5	K	247	SER
4	G	311	LEU
5	N	26	LEU
5	N	33	LEU
5	N	40	LEU
5	N	46	LEU
5	N	81	LYS
5	N	82	ILE
5	N	83	SER
5	N	85	LEU
5	N	87	LYS
5	N	93	ARG
5	N	99	LEU
5	N	106	LEU
5	N	107	LYS
5	N	110	ARG
5	N	114	LEU
5	N	126	LYS
5	N	128	THR
5	N	149	THR
5	N	149(A)	THR
5	N	149(B)	SER
5	N	149(C)	VAL
5	N	149(E)	GLU
5	N	151	GLN
5	N	153	SER
5	N	157	VAL
5	N	164	GLU
5	N	174	ILE
5	N	176	ILE
5	N	205	ASN
5	N	241	VAL
5	N	244	ARG
5	N	245	LEU
4	I	309	ASP
4	I	311	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16)

such sidechains are listed below:

Mol	Chain	Res	Type
1	L	13	GLN
2	H	60(G)	ASN
2	H	143	ASN
3	E	151	GLN
1	J	13	GLN
1	J	14(A)	GLN
5	K	71	HIS
1	M	13	GLN
1	M	14(A)	GLN
5	N	20	GLN
5	N	38	GLN
5	N	127	GLN
5	N	131	HIS
5	N	204(B)	ASN
5	N	205	ASN
5	N	239	GLN

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 oligosaccharides 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.