



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:44 AM UTC

PDB ID : 1HLT / pdb_00001hlt
Title : THE STRUCTURE OF A NONADECAPEPTIDE OF THE FIFTH EGF
DOMAIN OF THROMBOMODULIN COMPLEXED WITH THROMBIN
Authors : Tulinsky, A.; Mathews, I.I.
Deposited on : 1994-08-28
Resolution : 3.00 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

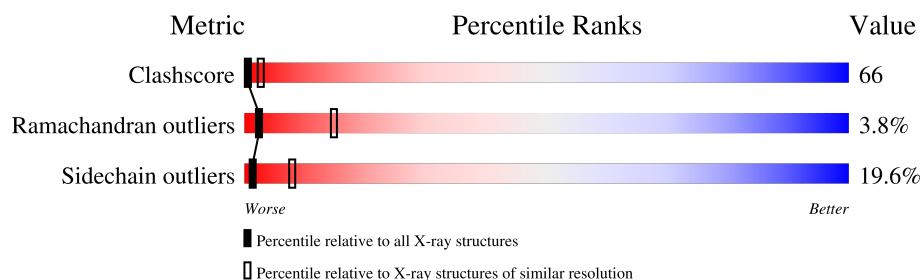
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	27	11% 56% 26% 7%
1	L	27	22% 44% 26% 7%
2	H	259	12% 47% 29% 8% .
2	K	259	15% 41% 34% 8% .
3	R	19	5% 21% 47% 16% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4756 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 ALPHA-THROMBIN (SMALL SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	27	Total	C	N	O	S	0	0	0
			218	136	36	45	1			
1	J	27	Total	C	N	O	S	0	0	0
			218	136	36	45	1			

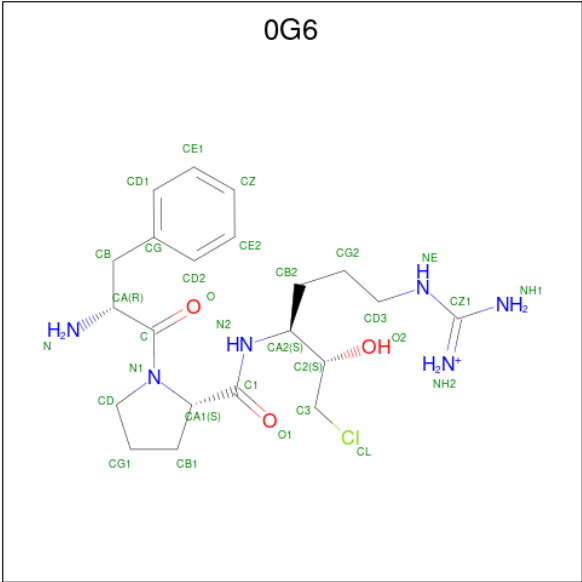
- Molecule 2 is a protein called ALPHA-THROMBIN (LARGE SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	251	Total	C	N	O	S	0	0	0
			2007	1279	353	361	14			
2	K	251	Total	C	N	O	S	0	0	0
			2007	1279	353	361	14			

- Molecule 3 is a protein called Thrombomodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	17	Total	C	N	O	S	0	0	0
			125	80	17	27	1			

- Molecule 4 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-prolinamide (CCD ID: 0G6) (formula: C₂₁H₃₄ClN₆O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			30	21	6	3		
4	K	1	Total	C	N	O	0	0
			30	21	6	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	6	Total	O	0	0
			6	6		
5	H	44	Total	O	0	0
			44	44		
5	J	6	Total	O	0	0
			6	6		
5	K	64	Total	O	0	0
			64	64		
5	R	1	Total	O	0	0
			1	1		

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.

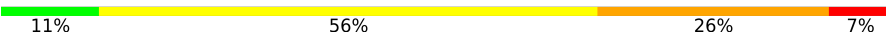
Note EDS was not executed.

• Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L: 

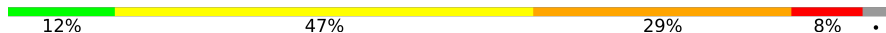


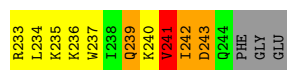
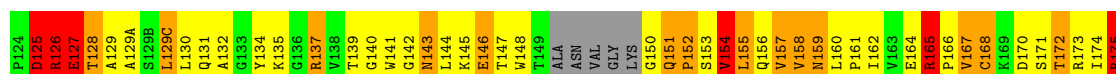
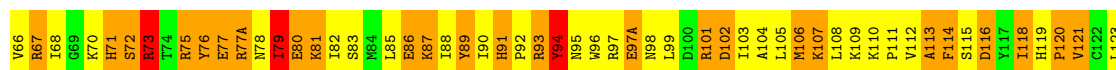
• Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain J: 

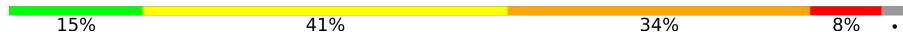


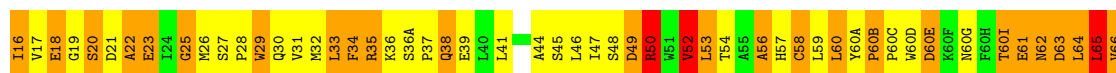
• Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

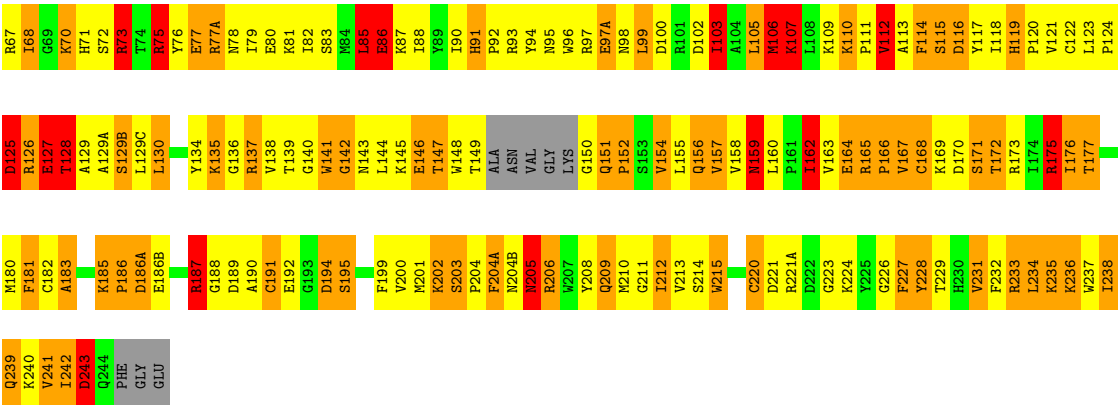
Chain H: 



• Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain K: 





● Molecule 3: Thrombomodulin



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	50.90 Å 50.90 Å 325.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.146 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4756	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: 0G6

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	1.33	1/220 (0.5%)	2.71	18/292 (6.2%)
1	L	1.49	0/220	2.51	16/292 (5.5%)
2	H	1.46	9/2058 (0.4%)	2.54	159/2783 (5.7%)
2	K	1.45	10/2058 (0.5%)	2.58	164/2783 (5.9%)
3	R	1.51	1/127 (0.8%)	3.31	24/172 (14.0%)
All	All	1.45	21/4683 (0.4%)	2.59	381/6322 (6.0%)

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	J	0	1
2	H	0	5
2	K	0	4
All	All	0	10

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	43	GLY	C-N	-7.13	1.23	1.33
2	H	33	LEU	N-CA	7.05	1.54	1.46
2	H	21	ASP	N-CA	6.04	1.53	1.46
2	K	114	PHE	N-CA	5.89	1.53	1.46
2	K	77(A)	ARG	NE-CZ	5.78	1.39	1.33
1	J	7	PHE	N-CA	5.68	1.53	1.46
2	K	211	GLY	N-CA	5.67	1.50	1.44
2	H	219	GLY	N-CA	5.65	1.54	1.45
2	H	77(A)	ARG	C-O	5.56	1.30	1.24
2	K	206	ARG	CD-NE	5.54	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	113	ALA	C-O	5.41	1.30	1.24
2	K	142	GLY	N-CA	5.35	1.51	1.45
2	K	191	CYS	N-CA	5.35	1.53	1.46
2	K	125	ASP	C-O	5.25	1.30	1.23
2	K	79	ILE	CA-CB	5.22	1.60	1.54
2	H	189	ASP	N-CA	-5.19	1.39	1.46
2	H	142	GLY	N-CA	5.19	1.49	1.44
2	H	95	ASN	C-N	5.13	1.41	1.33
2	K	33	LEU	N-CA	5.09	1.52	1.46
2	H	140	GLY	N-CA	-5.08	1.39	1.45
3	R	410	PRO	C-O	5.01	1.29	1.23

All (381) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	181	PHE	CA-CB-CG	16.40	130.20	113.80
3	R	410	PRO	O-C-N	16.20	143.47	122.89
2	H	140	GLY	N-CA-C	15.78	133.51	110.63
2	K	21	ASP	CA-CB-CG	14.79	127.39	112.60
1	J	14(D)	ARG	NE-CZ-NH2	12.69	130.62	119.20
2	H	159	ASN	CA-CB-CG	12.64	125.24	112.60
2	H	243	ASP	CA-CB-CG	12.54	125.14	112.60
2	K	45	SER	CA-C-O	-12.33	106.48	120.66
1	L	14(D)	ARG	CD-NE-CZ	12.03	141.23	124.40
2	K	159	ASN	CA-CB-CG	11.99	124.59	112.60
2	K	157	VAL	CA-C-O	-11.90	110.30	121.72
3	R	419	PHE	CA-CB-CG	-11.89	101.91	113.80
2	K	112	VAL	CA-C-O	10.96	132.10	120.48
2	H	213	VAL	CA-C-O	-10.77	107.31	120.78
1	L	4	ARG	CD-NE-CZ	10.68	139.35	124.40
2	H	135	LYS	CA-C-N	10.64	134.18	122.69
2	H	135	LYS	C-N-CA	10.64	134.18	122.69
2	H	186(A)	ASP	CA-CB-CG	-10.52	102.08	112.60
2	H	181	PHE	CA-CB-CG	10.45	124.25	113.80
2	H	116	ASP	CA-CB-CG	10.44	123.04	112.60
1	J	1(A)	ASP	N-CA-C	-10.31	100.82	113.50
2	K	102	ASP	CA-CB-CG	-10.28	102.32	112.60
1	J	14(D)	ARG	CD-NE-CZ	10.26	138.77	124.40
2	K	114	PHE	CA-CB-CG	10.25	124.05	113.80
2	H	91	HIS	CA-CB-CG	-9.76	104.04	113.80
1	L	7	PHE	CA-CB-CG	9.72	123.52	113.80
2	H	212	ILE	CA-C-O	-9.63	110.54	120.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	65	LEU	CA-C-O	-9.58	110.35	120.70
2	K	212	ILE	CA-C-O	-9.31	110.25	120.67
2	H	102	ASP	CA-CB-CG	9.29	121.89	112.60
2	H	206	ARG	NE-CZ-NH2	-9.08	111.03	119.20
2	H	33	LEU	CB-CA-C	9.06	125.36	110.22
2	K	49	ASP	CA-CB-CG	-9.02	103.58	112.60
3	R	411	GLU	O-C-N	8.98	134.53	122.59
2	H	194	ASP	CA-CB-CG	8.93	121.53	112.60
2	K	128	THR	N-CA-C	-8.90	100.74	111.69
2	H	21	ASP	CB-CA-C	8.88	124.40	109.75
2	H	114	PHE	CA-CB-CG	8.84	122.64	113.80
2	H	93	ARG	CB-CA-C	8.79	123.36	111.14
2	H	113	ALA	CA-C-O	-8.71	110.25	120.62
2	K	73	ARG	CB-CG-CD	8.66	131.22	111.30
2	K	227	PHE	CA-CB-CG	-8.64	105.16	113.80
2	K	113	ALA	CA-C-O	-8.55	108.28	120.51
2	K	86	GLU	N-CA-C	-8.52	102.47	113.12
1	J	1(A)	ASP	N-CA-CB	8.46	122.97	110.53
2	K	73	ARG	CD-NE-CZ	-8.46	112.55	124.40
2	K	232	PHE	CA-CB-CG	-8.46	105.34	113.80
2	K	23	GLU	CA-C-O	-8.36	111.86	121.47
1	J	12	LEU	CA-C-N	8.31	134.39	122.09
1	J	12	LEU	C-N-CA	8.31	134.39	122.09
1	L	1(A)	ASP	N-CA-C	-8.21	103.40	113.50
1	J	10	LYS	N-CA-C	-8.19	103.29	113.20
2	K	113	ALA	N-CA-CB	-8.16	96.70	110.49
2	K	204(A)	PHE	CA-CB-CG	-8.14	105.66	113.80
2	K	160	LEU	O-C-N	8.13	127.66	121.88
2	K	206	ARG	CD-NE-CZ	-8.13	113.02	124.40
2	H	77(A)	ARG	N-CA-C	8.05	119.69	111.07
2	K	78	ASN	CA-CB-CG	-8.00	104.61	112.60
2	H	104	ALA	CA-C-N	7.94	134.19	122.99
2	H	104	ALA	C-N-CA	7.94	134.19	122.99
2	H	237	TRP	N-CA-C	-7.89	102.76	111.36
2	H	127	GLU	CB-CG-CD	7.86	125.97	112.60
2	K	224	LYS	CA-CB-CG	7.83	129.77	114.10
2	H	239	GLN	CB-CG-CD	7.82	125.90	112.60
2	K	186(A)	ASP	CA-CB-CG	7.73	120.33	112.60
2	H	199	PHE	CA-CB-CG	7.71	121.51	113.80
2	K	127	GLU	CB-CG-CD	7.70	125.69	112.60
2	K	62	ASN	CA-C-O	-7.67	110.98	119.34
2	K	78	ASN	OD1-CG-ND2	7.62	130.22	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	184	GLY	N-CA-C	7.62	120.02	110.96
2	H	181	PHE	CB-CA-C	7.60	124.07	110.16
2	H	157	VAL	CA-C-O	-7.60	113.03	121.92
2	H	60(E)	ASP	CA-CB-CG	7.59	120.19	112.60
1	L	4	ARG	NE-CZ-NH1	7.56	129.06	121.50
2	K	99	LEU	CA-C-O	-7.54	111.43	120.32
2	K	227	PHE	CA-C-O	-7.53	112.23	120.43
2	K	203	SER	CA-C-O	-7.52	112.28	119.80
1	L	14(D)	ARG	NE-CZ-NH1	7.52	129.02	121.50
2	K	22	ALA	CA-C-O	-7.51	112.75	121.16
2	K	114	PHE	O-C-N	-7.44	113.87	123.02
2	K	77(A)	ARG	NE-CZ-NH1	7.43	128.93	121.50
2	H	123	LEU	CB-CA-C	7.40	119.93	108.61
1	J	8	GLU	CA-CB-CG	7.39	128.87	114.10
2	H	201	MET	CA-C-N	7.38	132.24	122.42
2	H	201	MET	C-N-CA	7.38	132.24	122.42
2	K	190	ALA	N-CA-C	-7.38	99.90	110.59
2	H	27	SER	O-C-N	7.35	126.56	121.19
2	K	34	PHE	CA-CB-CG	7.31	121.11	113.80
2	H	86	GLU	N-CA-C	-7.30	102.97	112.68
2	H	205	ASN	CA-CB-CG	7.18	119.78	112.60
2	K	190	ALA	CA-C-N	-7.17	109.70	122.32
2	K	190	ALA	C-N-CA	-7.17	109.70	122.32
2	H	228	TYR	CA-C-O	-7.17	112.42	120.66
2	H	201	MET	CB-CA-C	7.15	123.83	109.68
2	H	60(B)	PRO	N-CA-C	7.07	119.33	110.70
2	H	60	LEU	N-CA-CB	-7.07	98.81	110.68
2	K	199	PHE	CA-CB-CG	7.06	120.86	113.80
2	K	33	LEU	CB-CA-C	7.06	122.11	110.74
2	K	165	ARG	O-C-N	7.05	129.43	121.32
2	H	143	ASN	CA-CB-CG	7.01	119.61	112.60
2	H	65	LEU	CA-C-O	-7.01	113.13	120.70
1	J	7	PHE	CA-CB-CG	6.98	120.78	113.80
2	H	101	ARG	NE-CZ-NH1	6.97	128.47	121.50
2	K	66	VAL	CA-C-O	-6.96	113.12	120.57
2	H	127	GLU	CA-C-N	6.95	130.16	120.29
2	H	127	GLU	C-N-CA	6.95	130.16	120.29
2	K	73	ARG	NE-CZ-NH1	-6.95	114.55	121.50
2	K	125	ASP	CA-C-O	-6.92	113.56	121.72
2	H	159	ASN	OD1-CG-ND2	-6.90	115.70	122.60
2	K	60(I)	THR	CA-CB-OG1	-6.90	99.25	109.60
2	K	110	LYS	CB-CA-C	6.89	120.27	108.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	176	ILE	O-C-N	6.87	130.83	122.72
2	H	152	PRO	CA-C-O	-6.83	113.53	121.86
2	K	91	HIS	CA-CB-CG	-6.78	107.02	113.80
1	J	14(E)	GLU	N-CA-C	-6.75	104.86	113.23
2	K	158	VAL	CA-C-O	-6.75	112.34	120.78
1	J	14(H)	GLU	N-CA-C	-6.74	104.93	113.01
2	K	123	LEU	CB-CA-C	6.72	118.53	108.86
2	K	177	THR	N-CA-CB	6.70	122.50	111.31
2	K	146	GLU	N-CA-CB	6.69	120.68	109.78
2	K	50	ARG	NE-CZ-NH2	-6.68	113.19	119.20
2	K	60	LEU	N-CA-CB	-6.67	99.32	110.32
1	J	14(D)	ARG	NE-CZ-NH1	-6.66	114.84	121.50
3	R	417	ASP	O-C-N	6.64	131.42	122.59
2	K	67	ARG	NE-CZ-NH2	6.64	125.17	119.20
3	R	408	GLU	CA-C-N	-6.62	105.64	121.80
3	R	408	GLU	C-N-CA	-6.62	105.64	121.80
3	R	412	GLY	O-C-N	6.62	131.31	122.70
2	K	35	ARG	CD-NE-CZ	-6.62	115.14	124.40
2	K	170	ASP	CA-CB-CG	6.61	119.21	112.60
2	K	157	VAL	CA-CB-CG1	6.60	121.62	110.40
2	H	154	VAL	CB-CA-C	6.60	122.52	110.71
2	H	77(A)	ARG	CA-C-N	-6.59	112.13	122.73
2	H	77(A)	ARG	C-N-CA	-6.59	112.13	122.73
2	H	239	GLN	OE1-CD-NE2	-6.58	116.02	122.60
2	K	19	GLY	CA-C-N	6.57	133.10	122.53
2	K	19	GLY	C-N-CA	6.57	133.10	122.53
2	H	72	SER	CA-C-N	6.56	129.07	120.28
2	H	72	SER	C-N-CA	6.56	129.07	120.28
2	H	29	TRP	CA-C-O	-6.54	110.56	119.12
2	H	188	GLY	O-C-N	6.53	131.19	122.70
2	K	60(I)	THR	N-CA-C	6.52	118.44	109.18
1	L	14(D)	ARG	N-CA-C	-6.49	104.29	111.82
2	H	221(A)	ARG	CA-CB-CG	6.49	127.09	114.10
2	K	175	ARG	NE-CZ-NH2	-6.49	113.36	119.20
2	H	234	LEU	N-CA-CB	-6.47	101.12	110.56
3	R	422	THR	CA-C-O	-6.45	113.35	120.38
2	K	49	ASP	CB-CG-OD2	6.44	133.21	118.40
2	H	44	ALA	O-C-N	6.40	129.70	123.04
2	K	78	ASN	CA-C-N	6.38	129.88	122.35
2	K	78	ASN	C-N-CA	6.38	129.88	122.35
2	K	239	GLN	CA-CB-CG	6.38	126.85	114.10
2	H	55	ALA	CA-C-N	6.38	129.11	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	55	ALA	C-N-CA	6.38	129.11	120.38
2	H	147	THR	CA-C-N	6.37	133.71	121.54
2	H	147	THR	C-N-CA	6.37	133.71	121.54
2	H	208	TYR	CA-C-O	-6.37	114.01	121.46
2	K	164	GLU	CG-CD-OE1	-6.37	103.75	118.40
3	R	415	LEU	CA-C-N	-6.34	113.35	122.67
3	R	415	LEU	C-N-CA	-6.34	113.35	122.67
2	K	20	SER	N-CA-CB	6.32	121.86	111.31
2	K	156	GLN	CA-C-N	-6.31	115.35	122.48
2	K	156	GLN	C-N-CA	-6.31	115.35	122.48
3	R	410	PRO	CA-C-N	6.30	133.58	121.54
3	R	410	PRO	C-N-CA	6.30	133.58	121.54
2	H	140	GLY	CA-C-O	6.30	128.30	121.87
2	H	94	TYR	CA-C-O	-6.30	113.18	120.49
2	H	137	ARG	CA-CB-CG	6.29	126.68	114.10
2	K	152	PRO	O-C-N	6.27	130.62	123.03
2	K	106	MET	CB-CA-C	6.26	121.04	109.70
2	H	19	GLY	O-C-N	6.24	128.60	122.92
2	H	80	GLU	CA-C-O	-6.24	114.94	121.55
3	R	422	THR	CA-C-N	-6.24	114.47	122.77
3	R	422	THR	C-N-CA	-6.24	114.47	122.77
2	K	115	SER	CA-C-O	-6.23	113.70	121.55
2	H	234	LEU	CB-CA-C	6.21	121.06	110.56
2	H	97(A)	GLU	CB-CG-CD	6.19	123.13	112.60
2	H	106	MET	CB-CA-C	6.19	120.90	109.70
1	J	13	GLU	CB-CA-C	-6.17	99.35	109.53
2	H	21	ASP	CA-CB-CG	6.17	118.77	112.60
2	H	146	GLU	N-CA-CB	6.17	119.31	110.06
2	H	103	ILE	O-C-N	6.16	129.85	123.20
2	H	243	ASP	CB-CA-C	6.15	121.64	111.31
2	H	33	LEU	N-CA-CB	-6.14	99.85	110.17
2	K	94	TYR	CA-C-O	-6.13	113.75	120.81
2	K	168	CYS	O-C-N	6.13	128.41	122.03
2	K	183	ALA	N-CA-CB	-6.13	100.04	111.13
2	K	187	ARG	CD-NE-CZ	-6.13	115.82	124.40
2	K	116	ASP	N-CA-C	-6.12	105.79	113.20
2	H	140	GLY	O-C-N	-6.12	116.58	123.61
2	K	172	THR	CA-C-O	6.12	128.58	121.49
2	H	44	ALA	CA-C-O	-6.11	114.59	121.25
2	K	60(E)	ASP	N-CA-CB	-6.10	102.42	113.10
3	R	422	THR	N-CA-CB	6.09	120.13	110.57
2	H	126	ARG	N-CA-C	-6.09	103.96	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	233	ARG	NE-CZ-NH2	-6.09	113.72	119.20
2	K	190	ALA	CA-C-O	-6.09	114.77	121.89
2	K	141	TRP	CA-C-N	-6.07	115.87	122.55
2	K	141	TRP	C-N-CA	-6.07	115.87	122.55
2	H	93	ARG	CA-CB-CG	-6.06	101.98	114.10
1	L	10	LYS	CB-CG-CD	6.06	125.23	111.30
2	K	147	THR	CA-C-O	6.06	128.20	120.57
2	H	73	ARG	O-C-N	6.05	128.53	122.12
2	H	77(A)	ARG	CA-C-O	-6.04	114.47	120.82
2	H	195	SER	CA-CB-OG	-6.04	99.02	111.10
2	K	45	SER	O-C-N	6.04	130.64	123.27
2	K	239	GLN	OE1-CD-NE2	-6.03	116.57	122.60
2	H	76	TYR	CA-C-O	-6.02	114.86	122.63
2	H	87	LYS	CA-C-N	6.00	132.77	121.97
2	H	87	LYS	C-N-CA	6.00	132.77	121.97
2	H	207	TRP	CA-C-O	-6.00	113.85	120.69
2	K	243	ASP	O-C-N	5.97	130.53	122.59
2	H	30	GLN	CA-CB-CG	5.97	126.03	114.10
2	H	204(A)	PHE	N-CA-C	5.96	120.69	111.56
2	H	34	PHE	N-CA-C	5.95	118.94	109.24
2	K	146	GLU	CB-CG-CD	5.93	122.68	112.60
2	K	205	ASN	N-CA-CB	-5.93	103.29	112.30
2	H	129	ALA	CA-C-O	5.92	127.02	120.63
2	H	158	VAL	CA-C-O	-5.90	113.40	120.78
2	H	29	TRP	O-C-N	5.89	131.12	122.39
2	K	224	LYS	CB-CA-C	5.89	119.81	109.80
2	K	91	HIS	CA-C-N	5.89	125.76	119.28
2	K	91	HIS	C-N-CA	5.89	125.76	119.28
2	K	105	LEU	O-C-N	5.89	130.54	123.36
2	K	50	ARG	O-C-N	5.89	128.78	121.84
2	K	77(A)	ARG	NH1-CZ-NH2	-5.88	111.65	119.30
2	K	129(B)	SER	N-CA-C	5.88	119.55	112.38
2	H	123	LEU	N-CA-C	-5.88	102.75	110.39
2	H	170	ASP	N-CA-C	-5.86	105.62	112.89
2	K	115	SER	CA-CB-OG	5.86	122.83	111.10
3	R	424	ILE	CB-CG1-CD1	5.86	126.11	113.80
2	H	168	CYS	CA-C-N	5.85	129.20	120.31
2	H	168	CYS	C-N-CA	5.85	129.20	120.31
2	H	71	HIS	CA-CB-CG	5.84	119.64	113.80
2	K	221(A)	ARG	CA-CB-CG	5.80	125.70	114.10
2	K	23	GLU	CA-CB-CG	5.80	125.70	114.10
2	H	129(C)	LEU	O-C-N	5.79	128.71	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	204(B)	ASN	N-CA-C	-5.79	106.21	113.28
2	H	72	SER	O-C-N	5.79	129.82	123.22
2	K	228	TYR	CA-C-O	-5.78	114.63	121.16
2	H	139	THR	CA-C-N	5.77	130.10	121.04
2	H	139	THR	C-N-CA	5.77	130.10	121.04
2	H	146	GLU	N-CA-C	-5.77	104.34	111.33
2	K	170	ASP	N-CA-C	-5.77	105.50	112.54
2	H	60(E)	ASP	O-C-N	5.77	131.93	122.70
3	R	414	ILE	N-CA-CB	-5.76	104.43	110.82
2	K	67	ARG	NE-CZ-NH1	-5.74	115.76	121.50
1	J	1	CYS	N-CA-C	5.74	118.38	110.35
2	K	163	VAL	CB-CA-C	5.73	120.69	111.29
2	K	60(B)	PRO	N-CA-C	5.72	117.68	110.70
1	L	14(D)	ARG	CG-CD-NE	5.72	124.58	112.00
2	H	243	ASP	O-C-N	-5.71	115.84	122.87
3	R	417	ASP	CA-CB-CG	-5.67	106.93	112.60
2	H	157	VAL	O-C-N	5.66	128.65	122.76
2	H	64	LEU	CA-C-N	5.66	131.43	122.94
2	H	64	LEU	C-N-CA	5.66	131.43	122.94
2	K	215	TRP	N-CA-C	5.65	116.54	108.74
2	K	128	THR	O-C-N	5.65	129.58	122.23
2	H	126	ARG	N-CA-CB	5.65	119.07	110.14
2	H	233	ARG	NE-CZ-NH1	5.64	127.14	121.50
2	H	140	GLY	CA-C-N	5.64	131.52	122.83
2	H	140	GLY	C-N-CA	5.64	131.52	122.83
2	K	47	ILE	O-C-N	5.64	128.37	122.17
2	K	176	ILE	CA-C-O	-5.64	114.86	121.80
1	L	9	LYS	CB-CA-C	5.64	121.64	110.42
2	K	136	GLY	N-CA-C	-5.64	102.70	112.06
2	H	78	ASN	OD1-CG-ND2	5.63	128.23	122.60
2	K	189	ASP	CA-CB-CG	-5.62	106.97	112.60
2	H	120	PRO	N-CA-C	5.62	120.12	111.57
2	H	207	TRP	O-C-N	5.62	129.62	123.04
2	H	95	ASN	CA-C-N	-5.62	110.97	120.58
2	H	95	ASN	C-N-CA	-5.62	110.97	120.58
1	L	11	SER	CA-C-N	5.61	132.24	122.81
1	L	11	SER	C-N-CA	5.61	132.24	122.81
2	K	107	LYS	O-C-N	5.58	129.86	123.27
2	K	162	ILE	CA-C-O	-5.57	114.41	120.71
2	K	85	LEU	CA-C-O	5.56	127.03	120.69
2	K	30	GLN	CA-C-O	-5.56	115.39	120.95
2	K	49	ASP	CB-CG-OD1	-5.54	105.66	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	77(A)	ARG	CD-NE-CZ	5.54	132.16	124.40
2	H	233	ARG	CA-C-O	5.53	126.18	119.38
2	K	86	GLU	CA-C-O	-5.52	113.10	119.78
2	K	157	VAL	N-CA-C	-5.51	101.46	109.29
2	K	127	GLU	CG-CD-OE1	5.51	131.07	118.40
2	K	205	ASN	CB-CA-C	5.51	120.21	111.51
2	K	93	ARG	CA-CB-CG	-5.49	103.12	114.10
2	H	232	PHE	O-C-N	-5.48	116.31	122.12
3	R	411	GLU	CA-C-N	5.48	132.15	121.41
3	R	411	GLU	C-N-CA	5.48	132.15	121.41
2	K	151	GLN	CA-C-O	5.46	126.33	120.05
2	H	156	GLN	OE1-CD-NE2	5.45	128.05	122.60
1	J	14	ASP	CB-CA-C	5.44	119.36	109.83
1	J	14(C)	GLU	CG-CD-OE1	-5.43	105.91	118.40
2	K	107	LYS	N-CA-CB	5.43	119.07	110.55
2	H	79	ILE	O-C-N	5.42	129.35	122.57
2	H	62	ASN	CA-C-O	-5.41	113.09	119.48
1	J	14(B)	THR	CA-CB-CG2	5.40	119.68	110.50
2	H	121	VAL	CA-CB-CG2	5.40	119.57	110.40
2	K	63	ASP	N-CA-C	-5.39	105.37	113.89
3	R	422	THR	N-CA-C	-5.39	100.39	109.07
2	H	58	CYS	N-CA-C	-5.39	106.84	113.41
2	K	231	VAL	CA-CB-CG1	5.39	119.56	110.40
2	H	45	SER	O-C-N	5.38	130.06	123.44
2	K	224	LYS	N-CA-C	-5.38	98.80	108.48
2	K	119	HIS	CB-CA-C	5.38	116.64	109.65
2	K	175	ARG	NH1-CZ-NH2	5.38	126.29	119.30
2	K	38	GLN	OE1-CD-NE2	5.37	127.97	122.60
3	R	418	GLY	N-CA-C	-5.36	100.47	113.18
2	K	56	ALA	N-CA-C	5.36	117.12	111.28
2	K	209	GLN	N-CA-CB	5.35	119.14	110.42
2	K	234	LEU	N-CA-C	-5.35	105.40	112.94
2	K	202	LYS	CA-C-N	5.34	127.83	120.67
2	K	202	LYS	C-N-CA	5.34	127.83	120.67
2	K	180	MET	CA-C-O	-5.34	115.47	121.40
2	H	175	ARG	NE-CZ-NH1	5.33	126.83	121.50
2	K	243	ASP	CA-CB-CG	5.33	117.93	112.60
2	H	129(C)	LEU	N-CA-C	-5.32	107.44	114.31
2	K	52	VAL	N-CA-CB	-5.32	102.72	111.45
1	L	14(G)	LEU	CB-CA-C	5.31	120.77	110.46
1	J	14(E)	GLU	CB-CG-CD	5.31	121.63	112.60
2	H	127	GLU	CG-CD-OE1	5.31	130.61	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	17	VAL	CB-CA-C	-5.29	104.89	111.08
2	H	93	ARG	N-CA-CB	-5.29	102.96	110.79
2	H	225	TYR	CB-CA-C	5.29	119.23	109.71
2	K	231	VAL	O-C-N	5.27	127.26	121.83
2	H	182	CYS	CB-CA-C	5.26	119.70	109.33
2	K	32	MET	N-CA-CB	5.26	119.20	110.52
2	K	235	LYS	CA-C-O	-5.26	113.12	119.49
1	L	4	ARG	O-C-N	5.25	126.18	121.35
2	H	60(E)	ASP	CA-C-O	-5.25	114.47	120.98
1	L	14(D)	ARG	N-CA-CB	5.24	118.41	110.28
2	H	200	VAL	CA-C-O	5.23	125.81	121.68
2	K	234	LEU	O-C-N	5.23	128.52	122.19
2	K	204	PRO	CB-CA-C	5.21	118.90	111.04
2	H	125	ASP	CA-C-O	-5.20	115.29	121.16
2	K	114	PHE	CB-CA-C	5.19	118.80	110.29
2	K	220	CYS	N-CA-CB	5.18	119.25	110.49
2	H	47	ILE	N-CA-C	-5.18	107.78	113.43
2	H	129(C)	LEU	CB-CA-C	5.18	117.72	109.02
2	K	103	ILE	O-C-N	5.17	129.09	123.09
2	K	163	VAL	N-CA-CB	-5.17	102.70	111.23
2	K	58	CYS	N-CA-C	-5.17	105.72	112.23
2	H	209	GLN	OE1-CD-NE2	-5.16	117.44	122.60
2	H	123	LEU	CA-C-O	-5.16	115.32	120.63
2	H	161	PRO	CA-C-N	5.16	129.50	122.90
2	H	161	PRO	C-N-CA	5.16	129.50	122.90
2	K	60(B)	PRO	CB-CA-C	5.16	117.21	110.92
2	K	206	ARG	CG-CD-NE	-5.13	100.70	112.00
1	L	14(D)	ARG	NE-CZ-NH2	-5.13	114.58	119.20
2	K	165	ARG	N-CA-CB	5.13	119.50	110.37
2	K	29	TRP	CA-C-O	-5.13	114.07	119.97
2	K	137	ARG	CD-NE-CZ	5.13	131.58	124.40
2	H	35	ARG	N-CA-CB	5.13	117.89	109.95
2	H	58	CYS	O-C-N	5.12	129.64	122.36
2	K	107	LYS	CA-C-N	5.12	130.29	120.97
2	K	107	LYS	C-N-CA	5.12	130.29	120.97
2	K	185	LYS	CB-CA-C	5.12	116.79	109.11
2	H	168	CYS	N-CA-C	5.12	116.55	111.07
2	H	78	ASN	CB-CA-C	5.11	119.38	110.94
2	K	60(G)	ASN	CA-C-O	-5.11	113.20	120.51
2	K	119	HIS	CA-C-N	5.10	125.00	119.85
2	K	119	HIS	C-N-CA	5.10	125.00	119.85
2	H	24	ILE	CB-CG1-CD1	-5.10	103.09	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	159	ASN	CB-CG-ND2	5.09	124.04	116.40
3	R	423	ASP	CA-C-N	5.09	130.86	121.70
3	R	423	ASP	C-N-CA	5.09	130.86	121.70
2	K	238	ILE	O-C-N	5.08	127.18	121.94
2	H	241	VAL	O-C-N	5.08	126.80	121.87
2	K	25	GLY	CA-C-N	5.08	129.20	120.72
2	K	25	GLY	C-N-CA	5.08	129.20	120.72
2	K	136	GLY	CA-C-O	-5.06	116.11	121.88
2	H	180	MET	O-C-N	5.05	129.32	122.96
2	K	45	SER	N-CA-C	-5.05	100.81	109.24
2	K	77(A)	ARG	O-C-N	-5.05	116.77	122.12
2	H	65	LEU	N-CA-CB	-5.03	102.08	110.83
2	H	206	ARG	CG-CD-NE	-5.03	100.94	112.00
2	H	202	LYS	CB-CA-C	-5.02	102.52	110.81
2	H	187	ARG	NE-CZ-NH2	5.02	123.72	119.20
2	H	75	ARG	NE-CZ-NH1	5.02	126.52	121.50
2	H	199	PHE	N-CA-CB	5.01	118.95	110.69
2	H	93	ARG	NE-CZ-NH1	5.00	126.50	121.50

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	206	ARG	Sidechain
2	H	67	ARG	Sidechain
2	H	73	ARG	Sidechain
2	H	75	ARG	Sidechain
2	H	77(A)	ARG	Sidechain
1	J	14(D)	ARG	Sidechain
2	K	206	ARG	Sidechain
2	K	50	ARG	Sidechain
2	K	73	ARG	Sidechain
2	K	75	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	218	0	215	43	0
1	L	218	0	215	39	0
2	H	2007	0	1961	264	0
2	K	2007	0	1961	261	0
3	R	125	0	107	39	0
4	H	30	0	31	12	0
4	K	30	0	32	10	0
5	H	44	0	0	2	0
5	J	6	0	0	1	0
5	K	64	0	0	4	0
5	L	6	0	0	2	0
5	R	1	0	0	0	0
All	All	4756	0	4522	598	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 66.

All (598) 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)
2:H:195:SER:OG	4:H:1:0G6:H33	1.10	1.25
2:K:191:CYS:O	2:K:194:ASP:HB2	1.47	1.14
2:K:201:MET:CE	2:K:210:MET:HG3	1.78	1.13
2:K:195:SER:HG	4:K:1:0G6:C2	1.56	1.12
2:K:201:MET:HE3	2:K:210:MET:HG3	1.13	1.11
2:K:233:ARG:HH11	2:K:233:ARG:HG2	1.13	1.10
2:K:195:SER:OG	4:K:1:0G6:C3	2.00	1.10
2:K:107:LYS:HG2	2:K:107:LYS:O	1.51	1.09
1:J:14(F):LEU:O	1:J:14(I):SER:HB3	1.50	1.09
2:H:195:SER:HG	4:H:1:0G6:C2	1.57	1.07
1:J:6:LEU:HD12	2:K:25:GLY:HA3	1.32	1.06
2:H:126:ARG:NH1	2:H:127:GLU:HA	1.69	1.06
2:K:205:ASN:C	2:K:205:ASN:HD22	1.66	1.02
2:H:32:MET:HE3	2:H:70:LYS:HD3	1.40	1.01
2:K:200:VAL:HG12	2:K:209:GLN:HA	1.37	1.00
2:K:187:ARG:NH1	2:K:187:ARG:HG2	1.74	0.99
2:K:60(I):THR:HG22	2:K:61:GLU:H	1.25	0.99
1:L:14(A):LYS:CG	1:L:14(B):THR:HG23	1.93	0.98
2:K:91:HIS:HB2	2:K:103:ILE:HG23	1.46	0.97
2:K:18:GLU:HG3	2:K:187:ARG:HB2	1.43	0.96
2:K:195:SER:OG	4:K:1:0G6:H33	1.64	0.95
3:R:409:CYS:CB	3:R:410:PRO:HD2	1.97	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:415:LEU:HD13	3:R:422:THR:HB	1.46	0.94
2:K:107:LYS:O	2:K:107:LYS:CG	2.18	0.92
2:K:187:ARG:HG2	2:K:187:ARG:HH11	1.31	0.92
2:K:208:TYR:CB	2:K:210:MET:HE2	2.00	0.91
1:L:4:ARG:HG3	1:L:8:GLU:OE1	1.71	0.90
2:H:31:VAL:HB	2:H:44:ALA:HB3	1.53	0.90
2:K:204(B):ASN:H	2:K:204(B):ASN:HD22	1.15	0.90
2:K:139:THR:HG22	2:K:157:VAL:HA	1.52	0.90
2:K:60(I):THR:HG22	2:K:61:GLU:N	1.85	0.89
3:R:409:CYS:CB	3:R:410:PRO:CD	2.51	0.88
3:R:420:ILE:HD12	3:R:420:ILE:N	1.88	0.88
2:K:77(A):ARG:HH21	3:R:415:LEU:HD23	1.39	0.88
2:K:124:PRO:HB2	2:K:129:ALA:HB2	1.56	0.87
3:R:420:ILE:HD12	3:R:420:ILE:H	1.38	0.87
2:K:201:MET:HE3	2:K:210:MET:CG	2.02	0.87
1:J:6:LEU:HD21	2:K:116:ASP:HB3	1.55	0.87
2:K:233:ARG:HG2	2:K:233:ARG:NH1	1.88	0.87
2:K:183:ALA:HB3	2:K:228:TYR:HE2	1.40	0.86
2:K:205:ASN:O	2:K:205:ASN:ND2	2.08	0.86
2:H:67:ARG:NH1	2:H:70:LYS:HE2	1.91	0.85
2:K:125:ASP:OD2	2:K:128:THR:HB	1.75	0.85
2:H:97(A):GLU:OE1	2:H:175:ARG:HD3	1.78	0.84
1:J:14:ASP:HB2	2:K:23:GLU:OE2	1.76	0.84
1:L:14(A):LYS:HG3	1:L:14(B):THR:HG23	1.59	0.84
2:K:205:ASN:C	2:K:205:ASN:ND2	2.31	0.84
2:H:60:LEU:HD12	2:H:60(B):PRO:HD3	1.60	0.84
2:K:236:LYS:HD3	2:K:236:LYS:N	1.93	0.84
2:K:168:CYS:O	2:K:171:SER:HB3	1.76	0.84
2:K:41:LEU:HD23	2:K:64:LEU:HD11	1.59	0.83
2:K:16:ILE:HD11	2:K:138:VAL:HG12	1.61	0.83
2:H:41:LEU:HD22	2:H:64:LEU:CD1	2.09	0.83
2:K:60(I):THR:CG2	2:K:61:GLU:H	1.93	0.81
2:K:208:TYR:HB3	2:K:210:MET:HE2	1.61	0.81
2:H:213:VAL:HG12	2:H:213:VAL:O	1.79	0.81
2:H:76:TYR:CD2	3:R:422:THR:HG21	2.16	0.80
2:H:205:ASN:ND2	2:H:205:ASN:O	2.13	0.80
2:H:73:ARG:HD3	2:H:152:PRO:O	1.82	0.79
1:L:14(A):LYS:HG2	1:L:14(B):THR:HG23	1.60	0.79
2:K:164:GLU:OE1	2:K:164:GLU:N	2.15	0.79
2:K:60:LEU:HD23	2:K:90:ILE:HD13	1.64	0.78
1:J:6:LEU:CD1	2:K:25:GLY:HA3	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:201:MET:CE	2:K:210:MET:CG	2.60	0.78
2:K:187:ARG:HH11	2:K:187:ARG:CG	1.91	0.78
2:H:126:ARG:NH1	2:H:127:GLU:CA	2.46	0.77
2:H:183:ALA:HB3	2:H:228:TYR:HE2	1.47	0.77
3:R:420:ILE:H	3:R:420:ILE:CD1	1.90	0.77
2:K:77(A):ARG:NH2	3:R:415:LEU:HD23	1.99	0.77
2:H:18:GLU:HG2	2:H:187:ARG:HB2	1.65	0.77
2:K:183:ALA:HB3	2:K:228:TYR:CE2	2.19	0.77
2:K:73:ARG:NH1	2:K:152:PRO:O	2.18	0.77
1:L:10:LYS:HZ3	1:L:10:LYS:HB3	1.49	0.77
2:H:215:TRP:CE3	4:H:1:OG6:HD2	2.20	0.76
1:L:9:LYS:O	1:L:11:SER:N	2.20	0.75
2:K:208:TYR:HB2	2:K:210:MET:HE2	1.67	0.75
2:H:67:ARG:HD2	2:H:70:LYS:HD2	1.66	0.75
1:J:14(F):LEU:HD13	2:K:159:ASN:OD1	1.86	0.75
2:K:33:LEU:HD11	2:K:106:MET:HE1	1.69	0.75
2:H:46:LEU:HD21	2:H:112:VAL:HG11	1.69	0.75
2:K:204(B):ASN:H	2:K:204(B):ASN:ND2	1.83	0.74
2:H:188:GLY:O	2:H:189:ASP:HB2	1.85	0.74
2:K:141:TRP:HA	2:K:152:PRO:HG2	1.70	0.73
2:H:22:ALA:HB3	2:H:155:LEU:HB3	1.68	0.73
2:H:41:LEU:HD22	2:H:64:LEU:HD11	1.69	0.73
2:H:77:GLU:O	2:H:80:GLU:HB3	1.89	0.73
2:K:60(A):TYR:CZ	2:K:60(C):PRO:HG2	2.23	0.73
1:L:4:ARG:NH1	2:H:207:TRP:HE1	1.86	0.72
2:K:37:PRO:O	2:K:39:GLU:HG2	1.88	0.72
2:K:237:TRP:O	2:K:241:VAL:HG22	1.88	0.72
2:H:32:MET:HE1	2:H:67:ARG:NH2	2.04	0.72
2:K:49:ASP:OD1	2:K:50:ARG:N	2.23	0.72
2:H:32:MET:HG3	2:H:141:TRP:CE3	2.25	0.72
2:H:46:LEU:HD11	2:H:48:SER:O	1.90	0.72
2:K:186:PRO:HG3	2:K:223:GLY:HA3	1.70	0.72
2:K:115:SER:HB2	2:K:117:TYR:H	1.54	0.72
2:K:144:LEU:HB2	2:K:150:GLY:O	1.89	0.72
1:J:4:ARG:NH2	1:J:14:ASP:OD2	2.23	0.71
2:H:32:MET:HE3	2:H:70:LYS:CD	2.20	0.71
2:H:235:LYS:O	2:H:239:GLN:HG3	1.90	0.71
2:H:60(I):THR:C	2:H:62:ASN:H	1.94	0.71
2:K:49:ASP:OD1	2:K:49:ASP:C	2.31	0.71
2:H:32:MET:HG3	2:H:141:TRP:CZ3	2.26	0.71
2:K:49:ASP:O	2:K:112:VAL:HG23	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:418:GLY:O	3:R:420:ILE:N	2.24	0.71
2:K:60(A):TYR:CE2	2:K:60(C):PRO:HG2	2.26	0.70
2:K:186:PRO:HG3	2:K:223:GLY:CA	2.21	0.70
2:H:67:ARG:CZ	2:H:70:LYS:HE2	2.21	0.70
2:H:76:TYR:HB3	3:R:415:LEU:CD1	2.21	0.70
2:K:236:LYS:N	2:K:236:LYS:CD	2.53	0.70
1:L:10:LYS:HB3	1:L:10:LYS:NZ	2.06	0.70
2:H:60(A):TYR:C	2:H:60(C):PRO:HD2	2.17	0.70
2:H:76:TYR:HB3	3:R:415:LEU:HD11	1.73	0.70
2:K:126:ARG:HH21	2:K:127:GLU:HB3	1.56	0.70
2:K:204(B):ASN:HD22	2:K:204(B):ASN:N	1.90	0.70
2:H:128:THR:O	2:H:129(C):LEU:HD12	1.92	0.69
2:K:73:ARG:HH11	2:K:73:ARG:CB	2.06	0.69
2:H:126:ARG:HH12	2:H:127:GLU:HA	1.55	0.69
2:H:76:TYR:CZ	3:R:424:ILE:HG21	2.27	0.69
2:K:41:LEU:CD2	2:K:64:LEU:HD11	2.21	0.69
2:H:29:TRP:O	2:H:45:SER:HA	1.93	0.69
2:H:51:TRP:CE3	2:H:105:LEU:HD22	2.27	0.69
2:H:129(C):LEU:HD21	2:H:204:PRO:HD2	1.74	0.69
2:K:77(A):ARG:NH1	3:R:417:ASP:HB2	2.08	0.69
1:L:14(A):LYS:NZ	1:L:14(B):THR:OG1	2.26	0.69
1:J:6:LEU:CD2	2:K:116:ASP:HB3	2.23	0.69
2:K:203:SER:OG	2:K:204(B):ASN:ND2	2.26	0.69
2:K:23:GLU:O	2:K:26:MET:HB2	1.93	0.68
2:H:85:LEU:CD1	2:H:88:ILE:HD11	2.23	0.68
2:K:60(B):PRO:HG2	2:K:96:TRP:CD2	2.28	0.68
2:K:22:ALA:O	2:K:71:HIS:HE1	1.77	0.68
2:K:75:ARG:HB2	2:K:75:ARG:CZ	2.24	0.68
2:H:46:LEU:CD1	2:H:48:SER:O	2.42	0.68
1:J:14(A):LYS:HG3	1:J:14(B):THR:HG22	1.75	0.68
2:H:186(A):ASP:OD1	2:H:186(A):ASP:N	2.26	0.68
2:K:53:LEU:HD11	2:K:103:ILE:HD11	1.76	0.68
2:H:80:GLU:HG3	2:H:81:LYS:N	2.08	0.67
2:K:36:LYS:HG3	2:K:65:LEU:HD13	1.76	0.67
1:J:14(J):TYR:OH	2:K:201:MET:HG2	1.95	0.67
2:K:18:GLU:CG	2:K:187:ARG:HB2	2.21	0.67
2:H:67:ARG:NH1	2:H:70:LYS:CE	2.56	0.67
1:L:9:LYS:C	1:L:11:SER:N	2.51	0.67
2:K:36:LYS:O	2:K:38:GLN:HG2	1.95	0.67
2:K:195:SER:HG	4:K:1:OG6:H34	1.43	0.67
2:H:130:LEU:HD23	2:H:162:ILE:HD13	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:125:ASP:OD2	2:H:128:THR:HB	1.96	0.66
2:H:143:ASN:HA	2:H:150:GLY:O	1.95	0.66
2:K:109:LYS:O	2:K:110:LYS:HG3	1.95	0.66
2:K:35:ARG:O	2:K:38:GLN:HA	1.95	0.66
2:K:73:ARG:HH11	2:K:73:ARG:HB3	1.60	0.66
1:J:14(A):LYS:O	1:J:14(D):ARG:NH2	2.25	0.66
2:K:165:ARG:C	2:K:169:LYS:HE3	2.21	0.66
2:K:60(I):THR:HG22	2:K:61:GLU:HG2	1.77	0.66
2:H:51:TRP:CG	2:H:242:ILE:HD13	2.30	0.66
2:H:60(I):THR:C	2:H:62:ASN:N	2.54	0.66
2:H:195:SER:CB	4:H:1:OG6:C2	2.75	0.65
2:H:96:TRP:CZ2	2:H:97:ARG:NH2	2.64	0.65
2:H:126:ARG:NH1	2:H:127:GLU:OE1	2.28	0.65
2:H:182:CYS:HA	2:H:226:GLY:O	1.97	0.65
2:K:31:VAL:HG22	2:K:68:ILE:HG23	1.79	0.65
2:H:51:TRP:NE1	2:H:242:ILE:HG23	2.11	0.65
2:H:105:LEU:HD13	2:H:241:VAL:HG22	1.78	0.65
2:H:105:LEU:HD13	2:H:241:VAL:CG2	2.26	0.65
2:K:142:GLY:O	2:K:152:PRO:CD	2.45	0.65
2:K:29:TRP:O	2:K:46:LEU:N	2.28	0.65
2:H:235:LYS:O	2:H:235:LYS:HG2	1.96	0.64
2:K:26:MET:SD	2:K:157:VAL:HG11	2.36	0.64
1:J:14(D):ARG:H	1:J:14(D):ARG:HD3	1.62	0.64
2:K:26:MET:HE2	2:K:137:ARG:NH1	2.12	0.64
2:H:132:ALA:HA	2:H:162:ILE:O	1.97	0.64
2:K:142:GLY:O	2:K:152:PRO:HD3	1.97	0.64
2:K:70:LYS:NZ	2:K:77:GLU:OE1	2.31	0.64
2:K:77(A):ARG:HH12	3:R:417:ASP:HB2	1.62	0.64
2:H:16:ILE:HG12	2:H:194:ASP:OD2	1.97	0.64
2:H:60(B):PRO:HG2	2:H:96:TRP:CD2	2.33	0.64
2:H:201:MET:HE3	2:H:210:MET:HG3	1.80	0.64
2:K:172:THR:OG1	2:K:173:ARG:N	2.30	0.63
2:K:139:THR:CG2	2:K:157:VAL:HA	2.24	0.63
2:K:60(I):THR:C	2:K:62:ASN:H	2.05	0.63
2:H:134:TYR:N	2:H:134:TYR:HD1	1.97	0.63
2:K:144:LEU:N	2:K:150:GLY:O	2.26	0.63
2:K:125:ASP:N	2:K:125:ASP:OD1	2.31	0.63
2:K:125:ASP:CG	2:K:128:THR:HB	2.24	0.63
1:L:4:ARG:HH11	2:H:207:TRP:HE1	1.46	0.63
1:J:7:PHE:CE2	1:J:14:ASP:HB3	2.34	0.63
2:K:126:ARG:O	2:K:129(A):ALA:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:41:LEU:HD22	2:H:64:LEU:HD12	1.77	0.62
2:H:68:ILE:CG2	2:H:118:ILE:HG23	2.30	0.62
2:K:195:SER:HG	4:K:1:OG6:H33	1.46	0.62
2:K:97(A):GLU:OE1	2:K:175:ARG:NH1	2.30	0.62
2:K:233:ARG:HH11	2:K:233:ARG:CG	1.98	0.62
2:K:233:ARG:NH1	2:K:233:ARG:CG	2.59	0.62
2:H:73:ARG:HG3	2:H:141:TRP:HB3	1.81	0.62
2:K:202:LYS:HE3	2:K:205:ASN:O	1.99	0.62
2:K:140:GLY:O	2:K:156:GLN:HB2	2.00	0.62
1:L:6:LEU:HD23	1:L:10:LYS:HD2	1.82	0.62
2:H:81:LYS:NZ	2:H:113:ALA:HB3	2.14	0.62
2:H:199:PHE:HE1	2:H:201:MET:HE2	1.65	0.61
2:H:125:ASP:HB2	2:H:127:GLU:HG2	1.82	0.61
2:K:200:VAL:HG12	2:K:209:GLN:CA	2.22	0.61
2:H:126:ARG:HA	2:H:232:PHE:CZ	2.36	0.61
1:J:10:LYS:NZ	5:J:710:HOH:O	2.34	0.61
2:H:85:LEU:HD13	2:H:88:ILE:HD11	1.82	0.61
1:L:9:LYS:C	1:L:11:SER:H	2.09	0.61
2:K:185:LYS:C	2:K:186(A):ASP:H	2.09	0.61
2:K:195:SER:HA	2:K:213:VAL:HG12	1.83	0.61
2:H:195:SER:CB	4:H:1:OG6:C3	2.78	0.61
2:H:49:ASP:O	2:H:111:PRO:HA	2.01	0.60
2:K:139:THR:HB	2:K:155:LEU:HD11	1.83	0.60
2:H:172:THR:OG1	2:H:173:ARG:N	2.32	0.60
2:K:99:LEU:HD11	4:K:1:OG6:HA1	1.82	0.60
2:H:26:MET:O	2:H:26:MET:HG2	2.02	0.60
2:H:79:ILE:HG22	2:H:80:GLU:N	2.15	0.60
2:K:100:ASP:OD2	2:K:177:THR:HG21	2.01	0.60
2:K:18:GLU:CB	2:K:188:GLY:HA2	2.31	0.60
1:L:7:PHE:O	1:L:11:SER:N	2.35	0.60
2:H:67:ARG:CD	2:H:80:GLU:OE2	2.50	0.60
2:K:23:GLU:HA	5:K:727:HOH:O	2.01	0.60
2:K:53:LEU:HD11	2:K:103:ILE:CD1	2.32	0.60
2:H:37:PRO:O	2:H:39:GLU:HG2	2.02	0.60
2:K:95:ASN:HD21	2:K:97(A):GLU:HB3	1.67	0.59
2:H:126:ARG:HB2	2:H:232:PHE:HZ	1.67	0.59
2:H:36:LYS:O	2:H:38:GLN:HG2	2.03	0.59
2:K:60:LEU:HD12	2:K:60(B):PRO:HD3	1.84	0.59
2:H:34:PHE:HB3	2:H:65:LEU:HB3	1.84	0.59
2:H:125:ASP:O	2:H:126:ARG:C	2.45	0.59
2:H:166:PRO:O	2:H:167:VAL:C	2.46	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:195:SER:OG	4:H:1:OG6:C3	2.48	0.59
2:K:103:ILE:HG21	2:K:234:LEU:HD13	1.82	0.59
2:K:168:CYS:C	2:K:171:SER:HB3	2.27	0.59
2:H:22:ALA:CB	2:H:155:LEU:HB3	2.33	0.59
4:H:1:OG6:HD3	4:H:1:OG6:CD1	2.33	0.58
1:J:9:LYS:C	1:J:11:SER:H	2.11	0.58
2:H:134:TYR:N	2:H:134:TYR:CD1	2.71	0.58
2:H:174:ILE:HD12	2:H:215:TRP:CZ3	2.38	0.58
2:H:164:GLU:O	2:H:167:VAL:HB	2.03	0.58
2:H:125:ASP:C	2:H:127:GLU:N	2.57	0.58
2:H:231:VAL:HG13	2:H:232:PHE:N	2.18	0.58
2:H:114:PHE:HB3	2:H:118:ILE:O	2.03	0.58
1:J:7:PHE:HB3	1:J:12:LEU:O	2.03	0.58
2:H:153:SER:O	2:H:154:VAL:HG23	2.02	0.58
2:K:182:CYS:HA	2:K:226:GLY:O	2.03	0.58
2:K:236:LYS:HD3	2:K:236:LYS:H	1.65	0.58
3:R:418:GLY:O	3:R:420:ILE:HG13	2.03	0.58
2:H:68:ILE:HG22	2:H:118:ILE:HG23	1.86	0.57
2:K:31:VAL:HB	2:K:44:ALA:HB3	1.87	0.57
2:K:165:ARG:O	2:K:169:LYS:HG3	2.04	0.57
2:H:60(I):THR:N	2:H:63:ASP:OD2	2.36	0.57
2:H:184(A):TYR:HB3	2:H:186(B):GLU:HB2	1.86	0.57
2:K:145:LYS:O	2:K:146:GLU:C	2.48	0.57
2:H:126:ARG:HB2	2:H:232:PHE:CZ	2.39	0.57
1:J:14(F):LEU:O	1:J:14(I):SER:CB	2.38	0.57
2:K:18:GLU:HB3	2:K:188:GLY:HA2	1.87	0.57
2:K:39:GLU:O	2:K:39:GLU:HG3	2.05	0.57
3:R:416:ASP:O	3:R:416:ASP:CG	2.48	0.57
2:H:57:HIS:HE1	2:H:214:SER:O	1.87	0.57
2:K:33:LEU:HD11	2:K:106:MET:CE	2.35	0.57
1:L:6:LEU:HA	1:L:10:LYS:CD	2.34	0.56
2:K:242:ILE:O	2:K:242:ILE:HG22	2.05	0.56
2:H:204(B):ASN:OD1	2:H:206:ARG:HB2	2.05	0.56
1:L:4:ARG:NH2	1:L:14:ASP:OD2	2.38	0.56
1:L:14(G):LEU:HD11	2:H:202:LYS:HD3	1.87	0.56
2:H:60:LEU:CD1	2:H:60(B):PRO:HD3	2.32	0.56
2:H:98:ASN:ND2	2:H:175:ARG:O	2.30	0.56
1:L:7:PHE:CE1	2:H:26:MET:HA	2.40	0.56
2:H:42:CYS:HB3	2:H:195:SER:O	2.04	0.56
2:K:70:LYS:NZ	2:K:72:SER:O	2.36	0.56
1:L:6:LEU:HA	1:L:10:LYS:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:31:VAL:CG1	2:K:66:VAL:HG13	2.35	0.56
2:K:127:GLU:HA	2:K:129(A):ALA:HB3	1.87	0.56
2:H:189:ASP:OD1	2:H:190:ALA:N	2.39	0.56
2:K:88:ILE:HG12	2:K:106:MET:HB3	1.88	0.56
2:K:60(B):PRO:HG2	2:K:96:TRP:CE3	2.41	0.56
4:K:1:0G6:CD1	4:K:1:0G6:HD3	2.36	0.56
2:H:145:LYS:HB2	2:H:148:TRP:CB	2.36	0.55
1:J:14(J):TYR:CD1	2:K:134:TYR:CD2	2.94	0.55
2:K:33:LEU:O	2:K:41:LEU:HB3	2.06	0.55
2:K:29:TRP:CG	2:K:121:VAL:HB	2.41	0.55
2:K:130:LEU:HD23	2:K:201:MET:HE1	1.88	0.55
3:R:410:PRO:C	3:R:412:GLY:H	2.12	0.55
2:H:60(B):PRO:HG2	2:H:96:TRP:CE3	2.41	0.55
1:L:9:LYS:O	1:L:10:LYS:C	2.49	0.55
2:K:76:TYR:CD2	3:R:420:ILE:HD13	2.41	0.55
2:H:44:ALA:HB1	2:H:52:VAL:CG1	2.37	0.55
1:L:14(A):LYS:HG2	1:L:14(B):THR:N	2.21	0.55
2:H:57:HIS:CD2	2:H:57:HIS:O	2.59	0.55
2:H:145:LYS:HD3	2:H:148:TRP:CB	2.37	0.55
1:J:14(A):LYS:HZ2	1:J:14(B):THR:HG22	1.72	0.55
2:H:88:ILE:HG12	2:H:106:MET:CB	2.37	0.54
1:J:6:LEU:HD21	2:K:116:ASP:CB	2.31	0.54
2:K:59:LEU:HD11	2:K:106:MET:HE3	1.89	0.54
2:K:164:GLU:O	2:K:165:ARG:C	2.51	0.54
2:H:18:GLU:CG	2:H:187:ARG:HB2	2.35	0.54
2:H:20:SER:HB2	2:H:157:VAL:CG2	2.37	0.54
1:J:14(A):LYS:NZ	1:J:14(B):THR:HG22	2.22	0.54
2:K:58:CYS:SG	2:K:195:SER:HB2	2.47	0.54
2:K:139:THR:HG22	2:K:157:VAL:CA	2.31	0.54
2:K:195:SER:CB	4:K:1:0G6:H33	2.37	0.54
1:L:14(I):SER:OG	2:H:134:TYR:HA	2.08	0.54
2:H:76:TYR:HD2	3:R:422:THR:HG21	1.69	0.54
1:J:14(I):SER:OG	2:K:135:LYS:N	2.34	0.54
2:H:125:ASP:OD1	2:H:125:ASP:N	2.40	0.54
2:H:215:TRP:HA	4:H:1:0G6:HB32	1.90	0.54
2:H:29:TRP:O	2:H:46:LEU:N	2.38	0.53
2:H:57:HIS:CE1	2:H:214:SER:O	2.62	0.53
2:H:54:THR:HG23	2:H:55:ALA:N	2.24	0.53
2:H:126:ARG:HH11	2:H:127:GLU:CA	2.19	0.53
2:H:56:ALA:HB1	2:H:90:ILE:HG23	1.90	0.53
2:H:66:VAL:O	2:H:82:ILE:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:53:LEU:CD1	2:K:103:ILE:HD11	2.38	0.53
2:H:41:LEU:CD2	2:H:64:LEU:HD11	2.37	0.53
2:H:98:ASN:HA	4:H:1:OG6:HZ	1.91	0.53
1:L:4:ARG:H	1:L:8:GLU:HB2	1.74	0.53
1:J:14(G):LEU:C	1:J:14(I):SER:H	2.16	0.53
3:R:420:ILE:N	3:R:420:ILE:CD1	2.53	0.53
2:H:89:TYR:CD1	2:H:89:TYR:N	2.77	0.53
2:K:60(A):TYR:CZ	4:K:1:OG6:HG2	2.44	0.53
2:K:212:ILE:HB	2:K:229:THR:HB	1.90	0.53
3:R:415:LEU:HD13	3:R:422:THR:CB	2.30	0.53
2:K:173:ARG:O	2:K:173:ARG:HG2	2.09	0.52
2:H:65:LEU:HD23	3:R:413:TYR:CE2	2.44	0.52
2:H:185:LYS:HB2	2:H:186(B):GLU:HG3	1.91	0.52
2:H:67:ARG:NE	3:R:413:TYR:OH	2.42	0.52
2:K:60(D):TRP:O	2:K:60(E):ASP:HB2	2.08	0.52
2:H:76:TYR:CE2	3:R:424:ILE:CG2	2.93	0.52
2:H:181:PHE:O	2:H:227:PHE:HA	2.10	0.52
2:H:31:VAL:CG1	2:H:66:VAL:HG13	2.40	0.52
2:K:49:ASP:O	2:K:112:VAL:N	2.39	0.52
2:K:235:LYS:O	2:K:235:LYS:HG2	2.09	0.52
2:K:56:ALA:HB2	2:K:103:ILE:O	2.10	0.52
2:K:240:LYS:C	2:K:242:ILE:N	2.67	0.52
2:H:38:GLN:NE2	3:R:414:ILE:H	2.08	0.52
2:H:129(C):LEU:HD21	2:H:204:PRO:CD	2.38	0.52
2:H:203:SER:O	2:H:205:ASN:HA	2.11	0.51
2:K:130:LEU:CD2	2:K:201:MET:HE1	2.40	0.51
2:K:17:VAL:O	2:K:18:GLU:HB2	2.10	0.51
2:H:67:ARG:HD3	2:H:80:GLU:OE2	2.10	0.51
2:K:60(A):TYR:C	2:K:60(C):PRO:HD2	2.35	0.51
2:K:36(A):SER:HA	2:K:37:PRO:C	2.36	0.51
2:K:60(I):THR:C	2:K:62:ASN:N	2.69	0.51
2:K:17:VAL:O	2:K:188:GLY:HA2	2.11	0.51
2:K:105:LEU:HD11	2:K:238:ILE:HG23	1.92	0.51
2:K:181:PHE:O	2:K:227:PHE:HA	2.10	0.51
2:K:203:SER:O	2:K:205:ASN:HA	2.10	0.51
2:H:36(A):SER:HA	2:H:37:PRO:C	2.35	0.51
2:H:109:LYS:C	2:H:110:LYS:HG2	2.35	0.50
1:J:14(G):LEU:C	1:J:14(I):SER:N	2.65	0.50
1:J:14(J):TYR:HD1	2:K:134:TYR:CD2	2.29	0.50
2:K:18:GLU:HB2	2:K:188:GLY:HA2	1.93	0.50
2:K:59:LEU:HD11	2:K:106:MET:CE	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:17:VAL:HG11	2:K:221:ASP:HB3	1.93	0.50
2:K:36(A):SER:O	2:K:36(A):SER:OG	2.30	0.50
2:K:155:LEU:HD12	2:K:156:GLN:H	1.77	0.50
1:J:14(A):LYS:NZ	1:J:14(B):THR:CG2	2.75	0.50
2:H:205:ASN:HD22	2:H:205:ASN:C	2.20	0.50
1:J:1:CYS:O	2:K:122:CYS:SG	2.70	0.50
2:K:99:LEU:HD12	2:K:215:TRP:HB3	1.93	0.50
2:K:238:ILE:O	2:K:242:ILE:HB	2.12	0.50
2:H:174:ILE:CG2	2:H:175:ARG:N	2.75	0.49
2:H:67:ARG:HH12	2:H:70:LYS:HE2	1.74	0.49
3:R:415:LEU:CD1	3:R:422:THR:HB	2.31	0.49
1:L:3:LEU:HG	2:H:206:ARG:CG	2.42	0.49
2:K:57:HIS:HA	2:K:60:LEU:O	2.12	0.49
2:K:204(B):ASN:ND2	5:K:731:HOH:O	2.45	0.49
3:R:418:GLY:C	3:R:420:ILE:N	2.70	0.49
1:L:10:LYS:NZ	1:L:10:LYS:CB	2.70	0.49
2:K:242:ILE:O	2:K:242:ILE:CG2	2.61	0.49
2:H:86:GLU:HB2	2:H:109:LYS:HA	1.95	0.49
2:H:94:TYR:HB2	2:H:101:ARG:O	2.13	0.49
1:J:7:PHE:O	1:J:11:SER:N	2.45	0.49
2:K:165:ARG:NH1	2:K:176:ILE:HG22	2.28	0.49
2:K:139:THR:HA	2:K:156:GLN:O	2.13	0.49
1:L:14(B):THR:HA	5:L:945:HOH:O	2.13	0.49
2:H:87:LYS:HB3	2:H:89:TYR:CE1	2.47	0.49
2:H:236:LYS:O	2:H:240:LYS:HB2	2.12	0.49
2:K:77(A):ARG:HH22	3:R:416:ASP:H	1.61	0.49
2:H:67:ARG:HD2	2:H:80:GLU:OE2	2.13	0.48
2:H:208:TYR:HB3	2:H:210:MET:HE2	1.95	0.48
2:K:75:ARG:HB2	2:K:75:ARG:NH2	2.27	0.48
2:H:70:LYS:HE3	2:H:72:SER:O	2.13	0.48
2:H:60(A):TYR:CZ	2:H:60(C):PRO:HG2	2.47	0.48
2:H:71:HIS:O	2:H:154:VAL:HA	2.14	0.48
2:H:165:ARG:HB2	2:H:166:PRO:HD3	1.94	0.48
2:K:60:LEU:CD2	2:K:90:ILE:HD13	2.39	0.48
2:K:173:ARG:HB3	5:K:743:HOH:O	2.14	0.48
3:R:416:ASP:O	3:R:416:ASP:OD1	2.31	0.48
2:H:17:VAL:HG22	2:H:144:LEU:O	2.13	0.48
2:H:146:GLU:HB2	2:H:220:CYS:HB2	1.96	0.48
1:J:14(A):LYS:HG2	2:K:23:GLU:OE2	2.14	0.48
2:K:165:ARG:N	2:K:166:PRO:HD2	2.27	0.48
2:H:141:TRP:HA	2:H:152:PRO:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:31:VAL:HG13	2:K:66:VAL:HG13	1.95	0.48
2:H:28:PRO:HB2	2:H:119:HIS:HB3	1.95	0.48
2:H:146:GLU:HA	2:H:220:CYS:HB2	1.95	0.48
2:K:201:MET:HE2	2:K:210:MET:HG3	1.88	0.48
1:L:14(D):ARG:HG2	1:L:14(H):GLU:OE2	2.14	0.48
2:H:44:ALA:HB1	2:H:52:VAL:HG12	1.96	0.48
2:H:99:LEU:HD12	2:H:215:TRP:HB3	1.95	0.48
2:K:35:ARG:NH1	2:K:37:PRO:HD2	2.29	0.48
2:H:68:ILE:HG21	2:H:118:ILE:HG23	1.96	0.47
2:K:130:LEU:HD22	2:K:162:ILE:CD1	2.44	0.47
1:L:7:PHE:CE2	1:L:14:ASP:HB3	2.49	0.47
2:H:38:GLN:HE22	3:R:414:ILE:H	1.62	0.47
2:H:125:ASP:C	2:H:127:GLU:H	2.22	0.47
2:H:190:ALA:O	2:H:191:CYS:HB2	2.14	0.47
1:J:14(A):LYS:HZ2	1:J:14(B):THR:CG2	2.28	0.47
2:K:71:HIS:NE2	2:K:154:VAL:CG1	2.78	0.47
2:K:91:HIS:CB	2:K:103:ILE:HG23	2.32	0.47
2:K:148:TRP:O	2:K:149:THR:C	2.56	0.47
2:H:16:ILE:HG21	2:H:158:VAL:HB	1.96	0.47
2:H:151:GLN:HA	2:H:152:PRO:HD3	1.80	0.47
2:H:186:PRO:HD3	2:H:223:GLY:HA2	1.97	0.47
1:J:5:PRO:HA	1:J:9:LYS:HD2	1.95	0.47
2:K:98:ASN:ND2	2:K:175:ARG:HB3	2.30	0.47
2:H:26:MET:HE2	2:H:137:ARG:NH1	2.29	0.47
2:H:88:ILE:HG12	2:H:106:MET:HB2	1.97	0.47
2:H:93:ARG:O	2:H:101:ARG:HD2	2.15	0.47
2:K:91:HIS:HB2	2:K:103:ILE:CG2	2.31	0.47
1:L:4:ARG:NH1	2:H:207:TRP:NE1	2.60	0.47
2:H:34:PHE:CG	3:R:413:TYR:OH	2.66	0.47
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.78	0.47
2:H:168:CYS:O	2:H:171:SER:OG	2.27	0.47
2:K:185:LYS:H	2:K:186(B):GLU:HG3	1.79	0.47
1:L:14(B):THR:O	1:L:14(E):GLU:HB3	2.15	0.46
2:H:98:ASN:ND2	2:H:175:ARG:HB3	2.31	0.46
2:K:57:HIS:HE1	2:K:214:SER:O	1.98	0.46
2:H:19:GLY:HA2	2:H:158:VAL:HG23	1.97	0.46
2:K:110:LYS:HA	2:K:111:PRO:HD3	1.84	0.46
2:K:115:SER:C	2:K:117:TYR:H	2.19	0.46
2:K:17:VAL:HG11	2:K:221:ASP:CB	2.45	0.46
2:K:60(B):PRO:O	2:K:60(C):PRO:C	2.57	0.46
2:K:86:GLU:HA	2:K:109:LYS:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:185:LYS:C	2:K:186(A):ASP:N	2.74	0.46
1:L:14(J):TYR:CD2	2:H:204:PRO:HG3	2.51	0.46
2:H:145:LYS:O	2:H:146:GLU:C	2.58	0.46
2:H:201:MET:CE	2:H:210:MET:HG3	2.45	0.46
2:K:49:ASP:O	2:K:111:PRO:HA	2.15	0.46
2:K:52:VAL:O	2:K:105:LEU:HD23	2.15	0.46
2:K:167:VAL:O	2:K:171:SER:CB	2.64	0.46
2:H:236:LYS:HD3	2:H:236:LYS:N	2.30	0.46
2:K:124:PRO:HD3	2:K:209:GLN:O	2.16	0.46
3:R:422:THR:HG23	3:R:424:ILE:HG23	1.98	0.46
2:H:33:LEU:HD22	2:H:41:LEU:HD23	1.98	0.46
2:H:183:ALA:HB3	2:H:228:TYR:CE2	2.39	0.46
2:K:240:LYS:O	2:K:243:ASP:OD1	2.34	0.46
2:H:68:ILE:HB	2:H:118:ILE:HD13	1.97	0.45
1:J:4:ARG:HD3	1:J:8:GLU:OE1	2.15	0.45
2:H:105:LEU:HD13	2:H:241:VAL:HG21	1.97	0.45
2:H:199:PHE:HE1	2:H:201:MET:CE	2.28	0.45
2:H:17:VAL:HG13	2:H:144:LEU:O	2.17	0.45
2:H:174:ILE:HG22	2:H:175:ARG:N	2.31	0.45
2:H:184(A):TYR:CE2	2:H:186(D):LYS:HB2	2.51	0.45
2:H:192:GLU:OE2	5:H:915:HOH:O	2.21	0.45
1:J:9:LYS:C	1:J:11:SER:N	2.70	0.45
2:K:71:HIS:NE2	2:K:154:VAL:HG11	2.32	0.45
2:H:40:LEU:HG	2:H:41:LEU:N	2.31	0.45
1:J:10:LYS:HB3	1:J:10:LYS:HE2	1.69	0.45
2:K:86:GLU:CB	2:K:109:LYS:HG2	2.47	0.45
2:K:213:VAL:HG22	2:K:228:TYR:HE1	1.82	0.45
2:H:30:GLN:OE1	2:H:198:PRO:HD2	2.15	0.45
2:H:51:TRP:HE3	2:H:105:LEU:HD22	1.80	0.45
2:H:67:ARG:NH2	2:H:70:LYS:HE2	2.31	0.45
2:K:85:LEU:HD23	2:K:106:MET:HB2	1.98	0.45
2:K:91:HIS:ND1	2:K:92:PRO:HD2	2.32	0.45
2:K:208:TYR:HB2	2:K:210:MET:CE	2.42	0.45
2:H:51:TRP:CD1	2:H:242:ILE:HD13	2.51	0.45
2:H:126:ARG:HD3	2:H:127:GLU:OE1	2.16	0.45
2:H:215:TRP:CD2	4:H:1:OG6:HD2	2.50	0.45
2:H:231:VAL:CG1	2:H:232:PHE:N	2.79	0.45
2:H:38:GLN:HE22	3:R:413:TYR:HA	1.81	0.45
2:H:126:ARG:HA	2:H:232:PHE:CE2	2.51	0.45
2:K:73:ARG:HG3	2:K:141:TRP:HB3	1.99	0.45
2:H:183:ALA:CB	2:H:228:TYR:HE2	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:29:TRP:CD2	2:H:121:VAL:HB	2.52	0.44
2:H:154:VAL:O	2:H:155:LEU:C	2.60	0.44
1:J:14(J):TYR:HE2	2:K:202:LYS:O	1.99	0.44
2:K:98:ASN:OD1	2:K:98:ASN:N	2.50	0.44
2:H:23:GLU:HB2	2:H:26:MET:HB2	1.99	0.44
2:K:38:GLN:OE1	5:K:764:HOH:O	2.21	0.44
2:H:173:ARG:HG2	2:H:173:ARG:O	2.17	0.44
2:K:138:VAL:HG12	2:K:139:THR:N	2.31	0.44
2:H:81:LYS:HZ3	2:H:113:ALA:HB3	1.83	0.44
2:H:91:HIS:CE1	2:H:93:ARG:H	2.35	0.44
2:H:125:ASP:O	2:H:127:GLU:N	2.50	0.44
2:H:17:VAL:HG21	2:H:220:CYS:HB3	2.00	0.44
2:H:64:LEU:HD22	2:H:64:LEU:N	2.33	0.44
2:H:80:GLU:OE2	2:H:82:ILE:CG1	2.66	0.44
2:K:98:ASN:O	2:K:99:LEU:HB2	2.18	0.44
2:H:217:GLU:OE1	2:H:224:LYS:HE2	2.18	0.44
2:K:70:LYS:HE2	2:K:80:GLU:OE2	2.18	0.44
2:K:99:LEU:CD1	2:K:215:TRP:HB3	2.48	0.44
2:K:204(A):PHE:CD1	2:K:204(A):PHE:N	2.84	0.44
2:H:76:TYR:CZ	3:R:424:ILE:CG2	2.99	0.44
2:H:141:TRP:CE2	2:H:155:LEU:HD13	2.52	0.44
2:H:184(A):TYR:CE2	2:H:186(D):LYS:CB	3.01	0.44
2:K:31:VAL:CG1	2:K:44:ALA:HB3	2.48	0.43
2:K:76:TYR:CD1	2:K:76:TYR:C	2.94	0.43
2:K:144:LEU:HD12	2:K:144:LEU:HA	1.83	0.43
2:H:80:GLU:CG	2:H:81:LYS:N	2.71	0.43
1:J:14(D):ARG:HD3	1:J:14(D):ARG:N	2.31	0.43
2:H:61:GLU:HG2	2:H:62:ASN:OD1	2.18	0.43
2:K:82:ILE:CD1	3:R:420:ILE:HG12	2.48	0.43
2:K:235:LYS:HE2	2:K:239:GLN:HE21	1.82	0.43
2:H:96:TRP:CH2	2:H:97:ARG:NH2	2.85	0.43
2:H:131:GLN:O	2:H:132:ALA:C	2.62	0.43
2:K:95:ASN:ND2	2:K:97(A):GLU:HB3	2.31	0.43
2:H:96:TRP:HZ2	2:H:97:ARG:NH2	2.13	0.43
2:H:157:VAL:HG23	2:H:157:VAL:O	2.19	0.43
1:J:14(J):TYR:CE2	2:K:202:LYS:O	2.72	0.43
2:K:22:ALA:HA	2:K:157:VAL:HG13	2.01	0.43
1:L:6:LEU:HD23	1:L:10:LYS:CD	2.47	0.43
1:L:14(J):TYR:OH	2:H:201:MET:HG2	2.18	0.43
2:K:141:TRP:O	2:K:151:GLN:OE1	2.37	0.43
2:K:97(A):GLU:CD	2:K:175:ARG:HD3	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:86:GLU:HB2	2:K:109:LYS:HG2	2.00	0.43
2:H:107:LYS:HG2	2:H:108:LEU:O	2.19	0.43
2:H:165:ARG:CB	2:H:166:PRO:CD	2.97	0.43
2:H:201:MET:HE3	2:H:210:MET:CG	2.47	0.43
2:K:31:VAL:CB	2:K:44:ALA:HB3	2.48	0.43
2:H:88:ILE:HG12	2:H:106:MET:HB3	2.00	0.42
2:K:240:LYS:O	2:K:241:VAL:C	2.61	0.42
1:L:1:CYS:O	2:H:206:ARG:HD3	2.19	0.42
1:L:14:ASP:OD1	1:L:14:ASP:C	2.62	0.42
2:H:98:ASN:HD22	2:H:175:ARG:HB3	1.84	0.42
2:H:99:LEU:HD11	4:H:1:OG6:HB21	2.01	0.42
2:H:200:VAL:HG12	2:H:208:TYR:O	2.20	0.42
2:K:61:GLU:OE1	2:K:87:LYS:HA	2.19	0.42
2:H:60(A):TYR:C	2:H:60(C):PRO:CD	2.90	0.42
2:H:144:LEU:HD23	2:H:144:LEU:HA	1.78	0.42
2:H:33:LEU:N	2:H:42:CYS:O	2.41	0.42
2:K:127:GLU:HA	2:K:129(A):ALA:CB	2.49	0.42
2:K:147:THR:O	2:K:147:THR:HG23	2.20	0.42
2:K:152:PRO:HB3	2:K:156:GLN:CG	2.50	0.42
1:L:3:LEU:HG	2:H:206:ARG:HG2	2.02	0.42
2:H:57:HIS:HD1	2:H:102:ASP:CG	2.28	0.42
2:H:92:PRO:C	2:H:93:ARG:HG2	2.44	0.42
1:J:3:LEU:HD23	1:J:3:LEU:HA	1.90	0.42
2:H:32:MET:HG2	2:H:40:LEU:CD1	2.49	0.42
2:H:185:LYS:HB3	2:H:186:PRO:HD2	2.02	0.42
2:H:82:ILE:HD13	3:R:413:TYR:CE2	2.55	0.42
2:H:155:LEU:HD12	2:H:155:LEU:HA	1.46	0.42
1:J:1:CYS:C	2:K:122:CYS:SG	3.02	0.42
1:J:5:PRO:C	1:J:7:PHE:N	2.75	0.42
2:K:129:ALA:O	2:K:130:LEU:HB2	2.20	0.42
1:L:6:LEU:HG	2:H:116:ASP:HB3	2.02	0.41
2:H:60(G):ASN:O	5:H:901:HOH:O	2.21	0.41
2:H:235:LYS:HE2	2:H:239:GLN:HE21	1.85	0.41
2:K:143:ASN:HD21	2:K:149:THR:CA	2.33	0.41
2:K:148:TRP:CB	2:K:150:GLY:N	2.83	0.41
2:H:130:LEU:HD23	2:H:130:LEU:HA	1.89	0.41
2:K:71:HIS:CE1	2:K:154:VAL:HG13	2.55	0.41
2:K:167:VAL:H	2:K:167:VAL:HG23	1.39	0.41
2:K:34:PHE:CE2	2:K:38:GLN:HB3	2.55	0.41
2:K:168:CYS:O	2:K:171:SER:CB	2.56	0.41
2:H:232:PHE:HA	2:H:235:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:57:HIS:CE1	2:K:214:SER:O	2.74	0.41
2:H:32:MET:HE3	2:H:70:LYS:CE	2.50	0.41
2:H:165:ARG:CB	2:H:166:PRO:HD3	2.51	0.41
2:H:185:LYS:HB3	2:H:186(A):ASP:OD1	2.21	0.41
2:H:185:LYS:C	2:H:186(A):ASP:N	2.79	0.41
2:H:225:TYR:CD1	2:H:225:TYR:N	2.89	0.41
2:H:98:ASN:OD1	2:H:98:ASN:N	2.53	0.41
2:H:191:CYS:O	2:H:192:GLU:C	2.63	0.41
2:H:216:GLY:O	4:H:1:OG6:N	2.54	0.41
2:K:73:ARG:NH1	2:K:73:ARG:HB3	2.30	0.41
2:K:195:SER:HA	2:K:213:VAL:O	2.20	0.41
3:R:418:GLY:C	3:R:420:ILE:H	2.28	0.41
1:L:4:ARG:O	1:L:5:PRO:C	2.64	0.41
1:L:12:LEU:HD12	5:L:910:HOH:O	2.20	0.41
2:H:76:TYR:CE1	2:H:82:ILE:HD11	2.55	0.41
2:H:114:PHE:CZ	2:H:120:PRO:HG3	2.55	0.41
2:H:186:PRO:HG3	2:H:223:GLY:HA3	2.03	0.41
2:K:36:LYS:CG	2:K:65:LEU:HD13	2.48	0.41
2:K:105:LEU:HD12	2:K:241:VAL:HG21	2.02	0.41
2:K:114:PHE:HD1	2:K:118:ILE:HG22	1.85	0.41
2:K:119:HIS:HA	2:K:120:PRO:HD3	1.97	0.41
2:K:151:GLN:HA	2:K:152:PRO:HD3	1.94	0.41
2:K:152:PRO:CB	2:K:156:GLN:HG2	2.51	0.41
2:K:215:TRP:CE3	4:K:1:OG6:HD2	2.56	0.41
2:H:171:SER:O	2:H:224:LYS:HE3	2.20	0.41
2:H:213:VAL:O	2:H:213:VAL:CG1	2.47	0.41
1:J:5:PRO:C	1:J:7:PHE:H	2.28	0.41
2:K:97(A):GLU:OE1	2:K:175:ARG:HD3	2.21	0.41
2:K:126:ARG:HE	2:K:126:ARG:C	2.29	0.41
2:K:148:TRP:O	2:K:149:THR:O	2.39	0.41
2:K:185:LYS:HB2	2:K:186(B):GLU:HG3	2.03	0.41
2:H:76:TYR:HD2	3:R:415:LEU:HD11	1.86	0.40
2:H:240:LYS:HA	2:H:243:ASP:OD1	2.21	0.40
2:H:126:ARG:O	2:H:126:ARG:HG2	2.21	0.40
2:K:28:PRO:HB2	2:K:119:HIS:HB3	2.03	0.40
2:K:41:LEU:HD23	2:K:64:LEU:CD1	2.42	0.40
2:H:87:LYS:HB3	2:H:89:TYR:HE1	1.85	0.40
2:H:127:GLU:O	2:H:129(A):ALA:HB3	2.22	0.40
1:J:1:CYS:O	1:J:1:CYS:SG	2.80	0.40
1:J:14(G):LEU:HA	1:J:14(G):LEU:HD23	1.66	0.40
2:K:59:LEU:HD23	2:K:88:ILE:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:49:ASP:OD1	2:H:49:ASP:N	2.37	0.40
2:H:60(I):THR:O	2:H:62:ASN:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	25/27 (93%)	17 (68%)	7 (28%)	1 (4%)	2	14
1	L	25/27 (93%)	17 (68%)	5 (20%)	3 (12%)	0	1
2	H	247/259 (95%)	209 (85%)	29 (12%)	9 (4%)	2	16
2	K	247/259 (95%)	212 (86%)	30 (12%)	5 (2%)	6	28
3	R	15/19 (79%)	8 (53%)	4 (27%)	3 (20%)	0	0
All	All	559/591 (95%)	463 (83%)	75 (13%)	21 (4%)	2	15

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1	CYS
2	K	77	GLU
3	R	419	PHE
1	L	10	LYS
1	L	14(A)	LYS
2	H	213	VAL
3	R	412	GLY
2	H	77	GLU
2	H	155	LEU
2	K	243	ASP
2	H	189	ASP
2	K	166	PRO

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Mol	Chain	Res	Type
2	H	61	GLU
2	H	167	VAL
1	J	14(A)	LYS
3	R	409	CYS
2	H	60(B)	PRO
2	H	165	ARG
2	H	223	GLY
2	K	186	PRO
2	K	167	VAL

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	24/25 (96%)	23 (96%)	1 (4%)	26	61
1	L	24/25 (96%)	22 (92%)	2 (8%)	10	37
2	H	214/225 (95%)	174 (81%)	40 (19%)	1	9
2	K	214/225 (95%)	165 (77%)	49 (23%)	1	5
3	R	13/17 (76%)	9 (69%)	4 (31%)	0	1
All	All	489/517 (95%)	393 (80%)	96 (20%)	1	8

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	ARG
1	L	10	LYS
2	H	16	ILE
2	H	18	GLU
2	H	32	MET
2	H	41	LEU
2	H	50	ARG
2	H	53	LEU
2	H	54	THR
2	H	59	LEU

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Mol	Chain	Res	Type
2	H	61	GLU
2	H	62	ASN
2	H	64	LEU
2	H	79	ILE
2	H	81	LYS
2	H	83	SER
2	H	89	TYR
2	H	94	TYR
2	H	107	LYS
2	H	115	SER
2	H	118	ILE
2	H	125	ASP
2	H	126	ARG
2	H	127	GLU
2	H	128	THR
2	H	151	GLN
2	H	154	VAL
2	H	159	ASN
2	H	160	LEU
2	H	165	ARG
2	H	172	THR
2	H	175	ARG
2	H	176	ILE
2	H	182	CYS
2	H	185	LYS
2	H	199	PHE
2	H	200	VAL
2	H	205	ASN
2	H	206	ARG
2	H	224	LYS
2	H	241	VAL
2	H	242	ILE
1	J	10	LYS
2	K	16	ILE
2	K	18	GLU
2	K	20	SER
2	K	27	SER
2	K	48	SER
2	K	52	VAL
2	K	53	LEU
2	K	54	THR
2	K	61	GLU

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Mol	Chain	Res	Type
2	K	63	ASP
2	K	64	LEU
2	K	65	LEU
2	K	68	ILE
2	K	70	LYS
2	K	75	ARG
2	K	81	LYS
2	K	83	SER
2	K	85	LEU
2	K	86	GLU
2	K	97	ARG
2	K	97(A)	GLU
2	K	103	ILE
2	K	106	MET
2	K	107	LYS
2	K	112	VAL
2	K	125	ASP
2	K	126	ARG
2	K	127	GLU
2	K	128	THR
2	K	129(B)	SER
2	K	129(C)	LEU
2	K	130	LEU
2	K	135	LYS
2	K	154	VAL
2	K	159	ASN
2	K	162	ILE
2	K	171	SER
2	K	175	ARG
2	K	187	ARG
2	K	192	GLU
2	K	194	ASP
2	K	195	SER
2	K	205	ASN
2	K	220	CYS
2	K	231	VAL
2	K	233	ARG
2	K	236	LYS
2	K	241	VAL
2	K	242	ILE
3	R	415	LEU
3	R	416	ASP

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Mol	Chain	Res	Type
3	R	419	PHE
3	R	420	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	38	GLN
2	H	78	ASN
2	H	143	ASN
2	H	156	GLN
2	H	205	ASN
2	H	239	GLN
2	K	38	GLN
2	K	71	HIS
2	K	78	ASN
2	K	143	ASN
2	K	156	GLN
2	K	204(B)	ASN
2	K	205	ASN
2	K	230	HIS
2	K	239	GLN

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	0G6	K	1	2	30,31,32	0.93	0	37,41,42	2.00	12 (32%)
4	0G6	H	1	2	30,31,32	1.18	4 (13%)	37,41,42	3.08	10 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	0G6	K	1	2	-	8/31/41/43	0/2/2/2
4	0G6	H	1	2	-	7/31/41/43	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	0G6	C1-N2	-2.87	1.27	1.34
4	H	1	0G6	CA2-N2	-2.57	1.42	1.46
4	H	1	0G6	CZ1-NE	2.39	1.37	1.33
4	H	1	0G6	CB1-CA1	-2.18	1.48	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	0G6	CA2-N2-C1	14.78	148.95	123.25
4	K	1	0G6	CB2-CA2-N2	5.52	117.46	110.30
4	H	1	0G6	CB2-CA2-N2	5.20	117.05	110.30
4	K	1	0G6	CA2-N2-C1	4.43	130.94	123.25
4	K	1	0G6	CG2-CB2-CA2	3.87	121.31	113.94
4	H	1	0G6	C1-CA1-N1	-3.62	102.62	112.50
4	K	1	0G6	O-C-N1	3.36	127.42	121.38
4	H	1	0G6	CB1-CA1-C1	3.07	117.75	111.21
4	H	1	0G6	C2-CA2-N2	3.03	116.41	110.90
4	H	1	0G6	O1-C1-CA1	-2.99	113.48	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	0G6	CB1-CA1-N1	2.96	107.36	103.02
4	K	1	0G6	O-C-CA	-2.78	114.49	119.61
4	H	1	0G6	O1-C1-N2	2.75	127.89	122.96
4	H	1	0G6	CG-CB-CA	2.62	119.49	114.13
4	H	1	0G6	O-C-N1	2.52	125.91	121.38
4	K	1	0G6	NH1-CZ1-NH2	-2.40	113.24	120.07
4	K	1	0G6	O2-C2-C3	-2.40	102.51	109.68
4	K	1	0G6	CA1-C1-N2	2.34	121.67	116.52
4	K	1	0G6	C2-CA2-N2	-2.24	106.83	110.90
4	K	1	0G6	C1-CA1-N1	-2.24	106.38	112.50
4	K	1	0G6	CB1-CA1-N1	2.15	106.17	103.02
4	K	1	0G6	CG1-CB1-CA1	2.01	108.34	104.14

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	0G6	O2-C2-CA2-N2
4	H	1	0G6	C3-C2-CA2-N2
4	H	1	0G6	O2-C2-CA2-CB2
4	H	1	0G6	N2-CA2-CB2-CG2
4	H	1	0G6	C2-CA2-CB2-CG2
4	K	1	0G6	O2-C2-CA2-N2
4	K	1	0G6	O2-C2-CA2-CB2
4	K	1	0G6	NH1-CZ1-NE-CD3
4	K	1	0G6	NH2-CZ1-NE-CD3
4	H	1	0G6	NE-CD3-CG2-CB2
4	K	1	0G6	C3-C2-CA2-N2
4	K	1	0G6	N2-CA2-CB2-CG2
4	H	1	0G6	C3-C2-CA2-CB2
4	K	1	0G6	C2-CA2-CB2-CG2
4	K	1	0G6	CG2-CD3-NE-CZ1

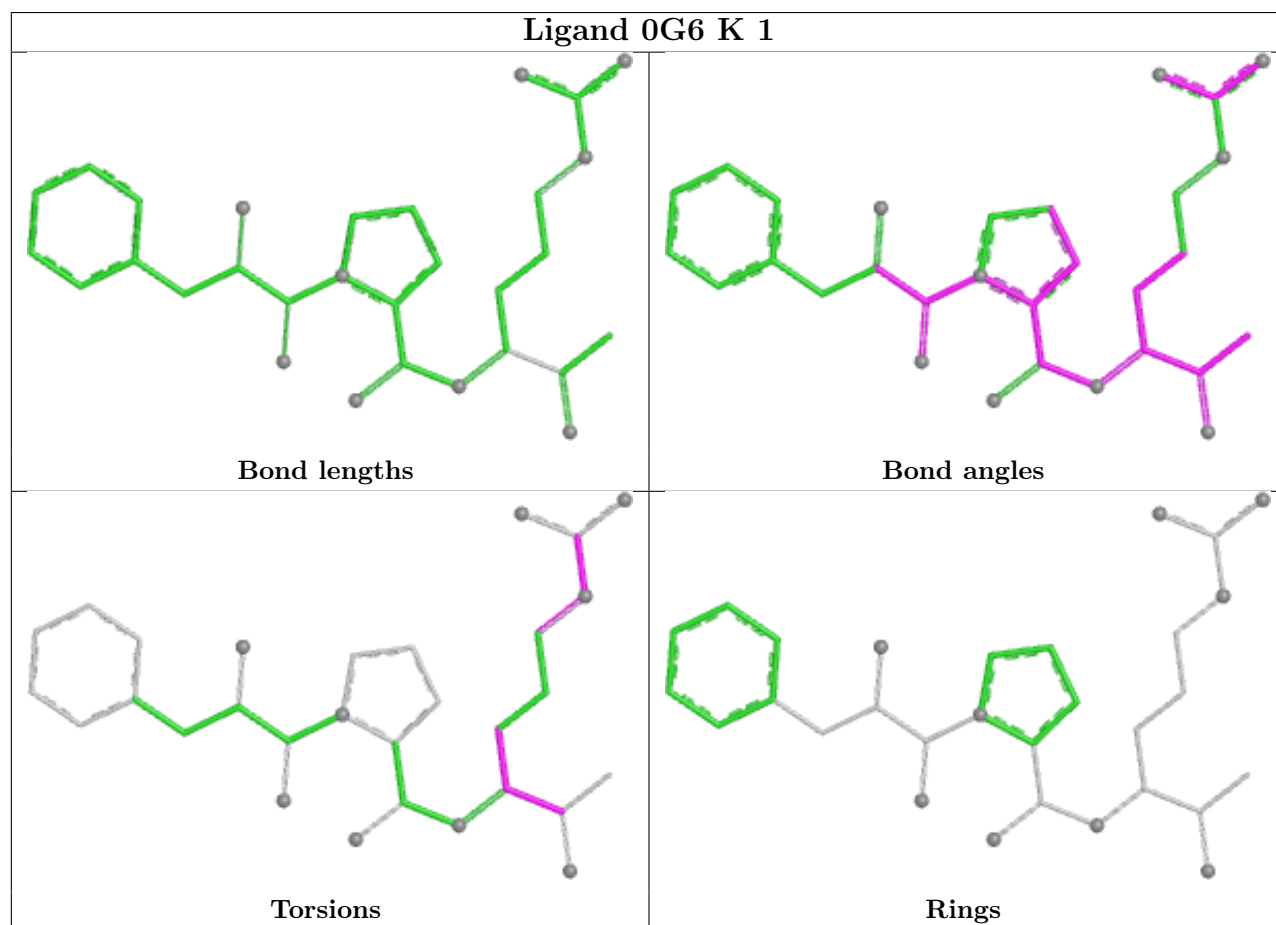
There are no ring outliers.

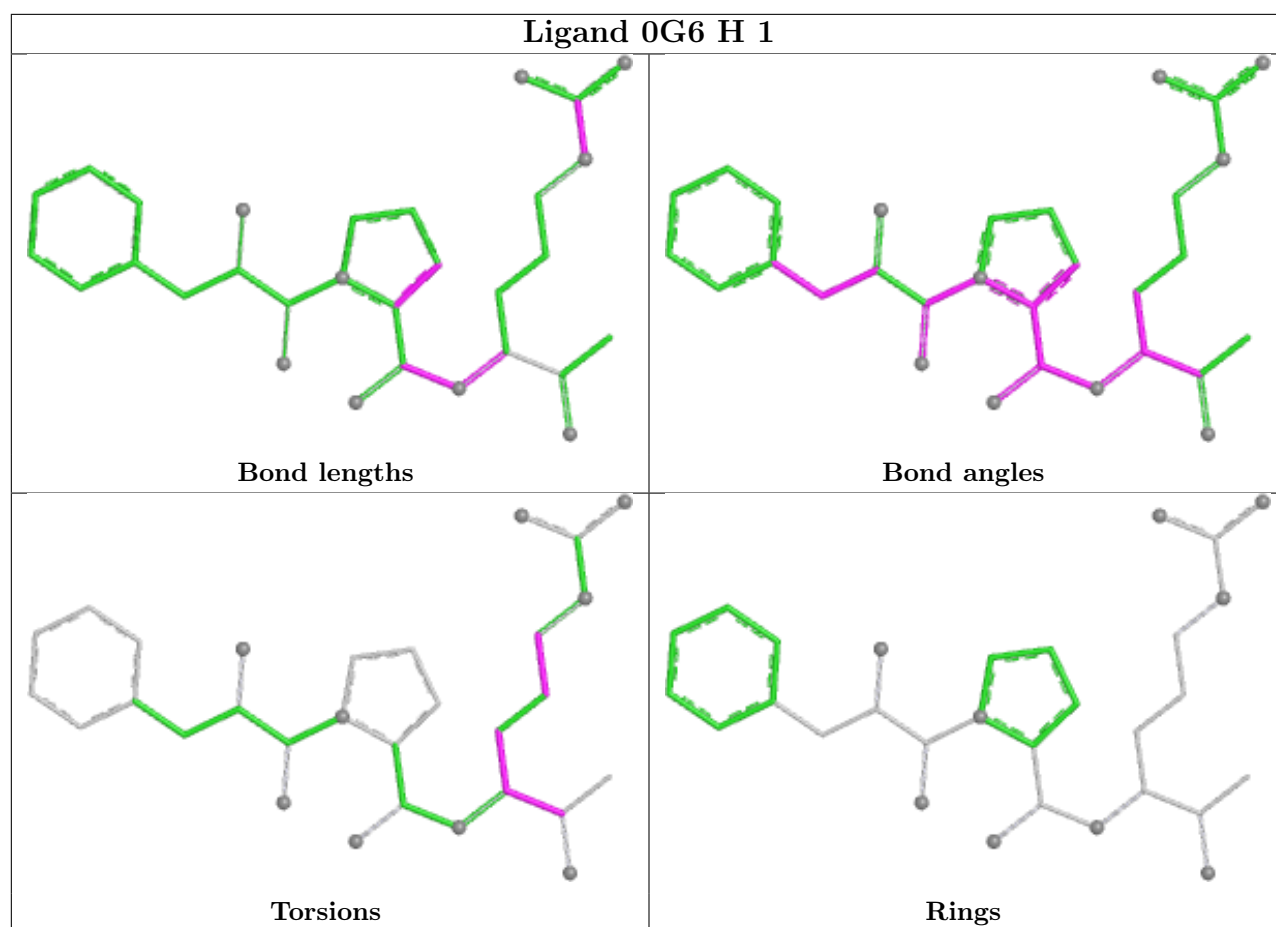
2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	0G6	10	0
4	H	1	0G6	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.