



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:51 PM GMT

PDB ID : 1HLT
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

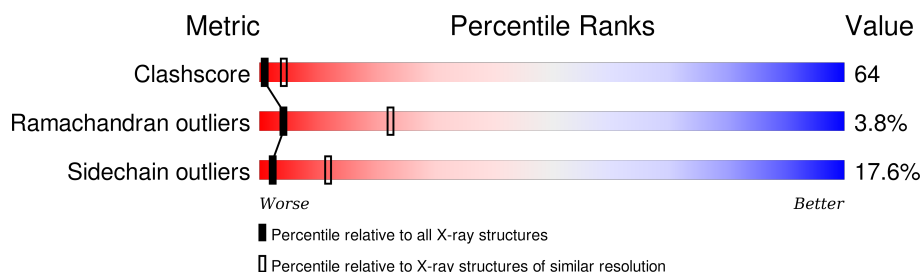
1 Overall quality at a glance

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	J	27	
1	L	27	
2	H	259	
2	K	259	
3	R	19	

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			

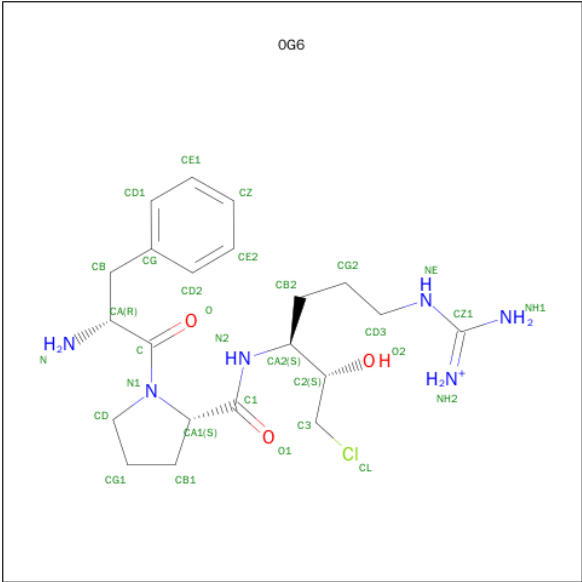
- Molecule 2 is a protein called ALPHA-THROMBIN (LARGE SUBUNIT).

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 (three-letter code: 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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

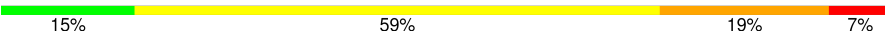
Note EDS was not executed.

- Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L: 



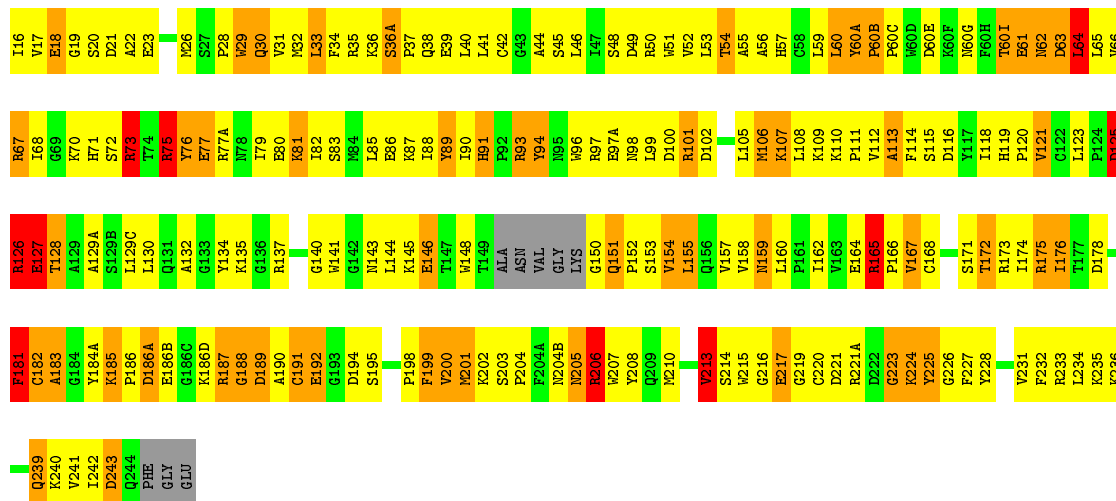
- Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain J: 



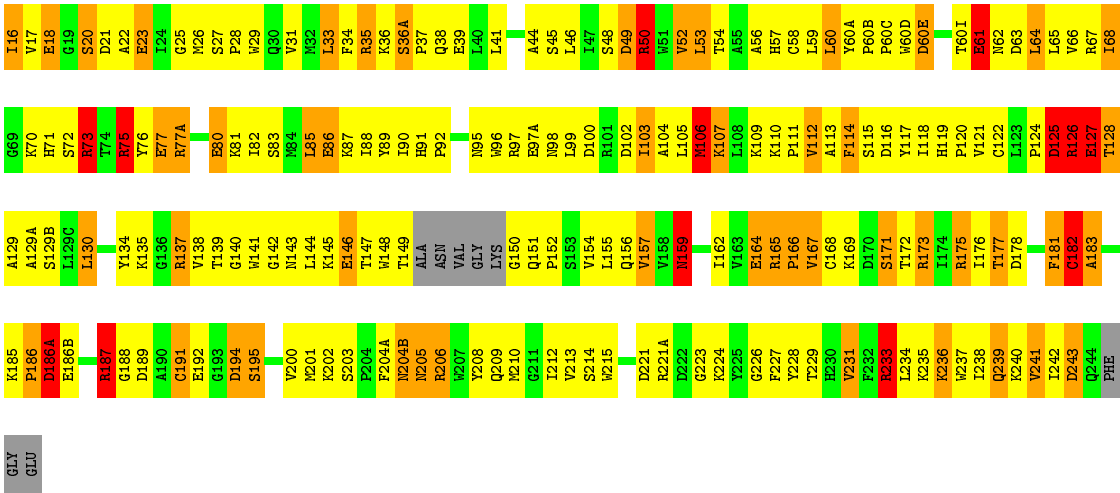
- Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H: 

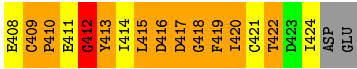


- Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain K: 



● Molecule 3: Thrombomodulin



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 [i](#)

5.1 Standard geometry [i](#)

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	1.20	0/220	2.54	11/292 (3.8%)
1	L	1.30	0/220	2.75	12/292 (4.1%)
2	H	1.15	3/2058 (0.1%)	2.12	76/2783 (2.7%)
2	K	1.13	0/2058	2.21	74/2783 (2.7%)
3	R	1.18	0/127	2.58	8/172 (4.7%)
All	All	1.15	3/4683 (0.1%)	2.23	181/6322 (2.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
2	H	0	5
2	K	0	4
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	219	GLY	N-CA	5.75	1.54	1.46
2	H	36(A)	SER	CB-OG	5.33	1.49	1.42
2	H	168	CYS	CB-SG	-5.30	1.73	1.81

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	14(D)	ARG	NE-CZ-NH2	20.65	130.62	120.30
2	H	206	ARG	NE-CZ-NH2	-18.54	111.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	4	ARG	NE-CZ-NH1	17.53	129.06	120.30
1	L	14(D)	ARG	NE-CZ-NH1	17.44	129.02	120.30
2	K	77(A)	ARG	NE-CZ-NH1	17.26	128.93	120.30
2	K	49	ASP	CB-CG-OD2	16.56	133.21	118.30
2	H	101	ARG	NE-CZ-NH1	16.34	128.47	120.30
2	K	50	ARG	NE-CZ-NH2	-14.22	113.19	120.30
2	K	49	ASP	CB-CG-OD1	-14.05	105.66	118.30
2	K	175	ARG	NE-CZ-NH2	-13.88	113.36	120.30
2	H	233	ARG	NE-CZ-NH1	13.69	127.14	120.30
2	H	233	ARG	NE-CZ-NH2	-13.16	113.72	120.30
2	H	175	ARG	NE-CZ-NH1	13.06	126.83	120.30
3	R	410	PRO	O-C-N	12.98	143.47	122.70
1	L	14(D)	ARG	CD-NE-CZ	12.60	141.23	123.60
2	H	75	ARG	NE-CZ-NH1	12.43	126.52	120.30
2	H	93	ARG	NE-CZ-NH1	12.41	126.50	120.30
2	K	50	ARG	NE-CZ-NH1	12.14	126.37	120.30
2	K	73	ARG	NE-CZ-NH1	-11.49	114.55	120.30
1	L	14(D)	ARG	NE-CZ-NH2	-11.44	114.58	120.30
1	L	4	ARG	CD-NE-CZ	11.25	139.35	123.60
1	J	14(D)	ARG	NE-CZ-NH1	-10.92	114.84	120.30
1	J	14(D)	ARG	CD-NE-CZ	10.84	138.77	123.60
2	H	93	ARG	NE-CZ-NH2	-10.81	114.90	120.30
2	K	97	ARG	NE-CZ-NH2	-10.74	114.93	120.30
2	K	165	ARG	NE-CZ-NH1	10.70	125.65	120.30
2	K	60(E)	ASP	CB-CG-OD2	10.20	127.48	118.30
2	H	243	ASP	CB-CG-OD1	9.90	127.21	118.30
2	H	175	ARG	NE-CZ-NH2	-9.88	115.36	120.30
2	K	67	ARG	NE-CZ-NH2	9.75	125.17	120.30
2	K	113	ALA	N-CA-CB	-9.57	96.70	110.10
2	K	186(A)	ASP	CB-CG-OD1	9.56	126.91	118.30
2	K	137	ARG	NE-CZ-NH2	-9.41	115.59	120.30
2	K	67	ARG	NE-CZ-NH1	-9.09	115.76	120.30
2	K	125	ASP	CB-CG-OD1	8.76	126.19	118.30
2	H	63	ASP	CB-CG-OD1	-8.72	110.45	118.30
3	R	410	PRO	CA-C-N	-8.36	98.81	117.20
2	H	60(A)	TYR	CB-CG-CD2	8.34	126.00	121.00
2	H	126	ARG	NE-CZ-NH1	8.16	124.38	120.30
2	H	140	GLY	N-CA-C	8.16	133.51	113.10
2	H	33	LEU	CB-CA-C	7.98	125.36	110.20
2	H	60(A)	TYR	CB-CG-CD1	-7.96	116.22	121.00
2	K	60(E)	ASP	CB-CG-OD1	-7.92	111.17	118.30
2	K	73	ARG	CD-NE-CZ	-7.89	112.55	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	189	ASP	CB-CG-OD1	-7.87	111.22	118.30
2	K	75	ARG	NE-CZ-NH2	-7.86	116.37	120.30
2	K	137	ARG	NE-CZ-NH1	7.78	124.19	120.30
2	K	53	LEU	CA-CB-CG	7.62	132.82	115.30
2	K	20	SER	N-CA-CB	7.58	121.86	110.50
2	K	206	ARG	CD-NE-CZ	-7.56	113.02	123.60
2	K	73	ARG	CB-CG-CD	7.54	131.22	111.60
2	K	80	GLU	OE1-CD-OE2	7.54	132.34	123.30
2	K	97	ARG	NE-CZ-NH1	7.53	124.07	120.30
2	K	224	LYS	CA-CB-CG	7.44	129.77	113.40
2	K	164	GLU	CG-CD-OE1	-7.27	103.75	118.30
2	K	183	ALA	N-CA-CB	-7.19	100.04	110.10
2	H	35	ARG	NE-CZ-NH2	-7.18	116.71	120.30
2	K	157	VAL	CA-CB-CG1	7.15	121.62	110.90
2	H	73	ARG	NE-CZ-NH2	-7.11	116.75	120.30
2	H	225	TYR	CB-CG-CD2	7.07	125.24	121.00
2	K	102	ASP	CB-CG-OD1	-7.05	111.95	118.30
2	K	77(A)	ARG	NH1-CZ-NH2	-7.05	111.65	119.40
1	J	8	GLU	CA-CB-CG	7.03	128.87	113.40
2	H	21	ASP	CB-CA-C	7.00	124.40	110.40
2	H	76	TYR	CB-CG-CD2	6.88	125.13	121.00
1	J	1(A)	ASP	N-CA-CB	6.87	122.97	110.60
2	K	206	ARG	NE-CZ-NH2	-6.85	116.87	120.30
2	H	181	PHE	CB-CA-C	6.84	124.07	110.40
2	H	187	ARG	NE-CZ-NH2	6.83	123.72	120.30
2	K	181	PHE	CA-CB-CG	6.79	130.20	113.90
2	H	53	LEU	CA-CB-CG	6.77	130.87	115.30
2	K	104	ALA	N-CA-CB	6.74	119.54	110.10
2	H	201	MET	CB-CA-C	6.71	123.83	110.40
3	R	411	GLU	O-C-N	6.67	134.53	123.20
1	L	1(A)	ASP	CB-CG-OD2	-6.62	112.34	118.30
2	H	73	ARG	NE-CZ-NH1	6.57	123.59	120.30
2	K	146	GLU	OE1-CD-OE2	-6.50	115.50	123.30
2	K	45	SER	CA-C-O	-6.48	106.48	120.10
2	H	93	ARG	CB-CA-C	6.48	123.36	110.40
3	R	408	GLU	C-N-CA	-6.42	105.64	121.70
2	K	177	THR	N-CA-CB	6.42	122.50	110.30
2	K	182	CYS	CA-CB-SG	6.41	125.54	114.00
2	K	127	GLU	CG-CD-OE1	6.38	131.07	118.30
2	H	125	ASP	CB-CG-OD2	6.37	124.03	118.30
2	K	21	ASP	CA-CB-CG	6.36	127.39	113.40
2	K	233	ARG	NE-CZ-NH2	-6.33	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	33	LEU	CA-CB-CG	6.29	129.77	115.30
2	K	33	LEU	CB-CA-C	6.27	122.11	110.20
2	K	173	ARG	NE-CZ-NH2	-6.27	117.17	120.30
2	K	175	ARG	NH1-CZ-NH2	6.26	126.29	119.40
2	K	89	TYR	CB-CG-CD1	6.26	124.76	121.00
2	H	102	ASP	CB-CG-OD1	6.24	123.91	118.30
2	H	221(A)	ARG	CA-CB-CG	6.22	127.09	113.40
1	J	14(C)	GLU	CG-CD-OE1	-6.19	105.91	118.30
2	H	127	GLU	CG-CD-OE1	6.15	130.61	118.30
2	K	239	GLN	CA-CB-CG	6.12	126.85	113.40
2	K	77(A)	ARG	CD-NE-CZ	6.11	132.16	123.60
1	L	13	GLU	OE1-CD-OE2	6.11	130.63	123.30
2	H	213	VAL	CA-C-O	-6.09	107.31	120.10
1	L	14(D)	ARG	CG-CD-NE	6.09	124.58	111.80
2	H	113	ALA	N-CA-CB	-6.06	101.62	110.10
2	K	35	ARG	CD-NE-CZ	-6.04	115.14	123.60
2	H	137	ARG	CA-CB-CG	6.04	126.68	113.40
2	H	63	ASP	CB-CG-OD2	5.96	123.66	118.30
1	L	4	ARG	NH1-CZ-NH2	-5.94	112.87	119.40
2	H	178	ASP	CB-CG-OD2	-5.88	113.01	118.30
2	H	186(A)	ASP	CB-CG-OD1	-5.87	113.02	118.30
2	H	154	VAL	CB-CA-C	5.85	122.52	111.40
2	H	127	GLU	OE1-CD-OE2	-5.85	116.28	123.30
2	K	178	ASP	CB-CG-OD2	-5.84	113.05	118.30
2	H	191	CYS	CA-CB-SG	5.83	124.48	114.00
2	H	60	LEU	N-CA-CB	-5.79	98.81	110.40
2	H	121	VAL	CA-CB-CG2	5.78	119.57	110.90
2	K	231	VAL	CA-CB-CG1	5.77	119.56	110.90
2	H	60(E)	ASP	O-C-N	5.77	131.93	122.70
2	K	187	ARG	NE-CZ-NH2	-5.77	117.42	120.30
2	H	178	ASP	CB-CG-OD1	5.76	123.48	118.30
2	H	30	GLN	CA-CB-CG	5.74	126.03	113.40
2	H	234	LEU	CB-CA-C	5.72	121.06	110.20
2	K	102	ASP	OD1-CG-OD2	5.72	134.16	123.30
2	K	112	VAL	CA-C-O	5.71	132.10	120.10
2	H	221	ASP	CB-CG-OD1	5.70	123.43	118.30
2	K	137	ARG	CD-NE-CZ	5.70	131.58	123.60
2	H	165	ARG	NE-CZ-NH2	5.68	123.14	120.30
2	K	173	ARG	NE-CZ-NH1	5.67	123.13	120.30
2	H	135	LYS	C-N-CA	5.66	134.18	122.30
2	H	101	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	H	91	HIS	CA-CB-CG	-5.63	104.04	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	113	ALA	CA-C-O	-5.63	108.28	120.10
2	H	243	ASP	CB-CA-C	5.62	121.64	110.40
1	L	9	LYS	CB-CA-C	5.62	121.64	110.40
2	K	191	CYS	CB-CA-C	5.61	121.62	110.40
2	K	146	GLU	N-CA-CB	5.60	120.68	110.60
2	K	221(A)	ARG	CA-CB-CG	5.59	125.70	113.40
2	K	23	GLU	CA-CB-CG	5.59	125.70	113.40
1	L	14(G)	LEU	CB-CA-C	5.56	120.77	110.20
2	K	126	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	K	187	ARG	CD-NE-CZ	-5.55	115.82	123.60
2	H	64	LEU	CA-CB-CG	5.55	128.06	115.30
2	K	60	LEU	N-CA-CB	-5.54	99.32	110.40
2	H	217	GLU	CG-CD-OE1	-5.53	107.25	118.30
1	J	13	GLU	CB-CA-C	-5.53	99.35	110.40
2	K	114	PHE	O-C-N	-5.52	113.87	122.70
2	H	102	ASP	CB-CG-OD2	-5.51	113.34	118.30
2	H	239	GLN	CB-CG-CD	5.50	125.90	111.60
2	H	100	ASP	CB-CG-OD1	5.49	123.24	118.30
2	H	146	GLU	CG-CD-OE2	5.45	129.21	118.30
2	H	183	ALA	N-CA-CB	-5.43	102.50	110.10
2	H	192	GLU	CG-CD-OE1	5.41	129.12	118.30
2	H	159	ASN	CA-CB-CG	5.38	125.24	113.40
3	R	412	GLY	O-C-N	5.38	131.31	122.70
2	H	243	ASP	CA-CB-CG	5.33	125.14	113.40
2	K	106	MET	CB-CA-C	5.32	121.04	110.40
2	H	225	TYR	CB-CG-CD1	-5.31	117.81	121.00
2	K	127	GLU	OE1-CD-OE2	-5.31	116.93	123.30
2	H	188	GLY	O-C-N	5.30	131.19	122.70
2	K	206	ARG	CG-CD-NE	-5.29	100.70	111.80
2	H	33	LEU	N-CA-CB	-5.28	99.85	110.40
2	H	29	TRP	O-C-N	5.26	131.12	122.70
2	H	76	TYR	CB-CG-CD1	-5.25	117.85	121.00
2	H	106	MET	CB-CA-C	5.25	120.90	110.40
1	L	10	LYS	CB-CG-CD	5.24	125.23	111.60
1	J	14(E)	GLU	CG-CD-OE1	5.24	128.78	118.30
1	J	14(B)	THR	CA-CB-CG2	5.20	119.68	112.40
2	H	93	ARG	CA-CB-CG	-5.19	101.98	113.40
1	J	14	ASP	CB-CG-OD1	-5.19	113.63	118.30
2	K	80	GLU	CG-CD-OE1	-5.18	107.94	118.30
3	R	422	THR	N-CA-CB	5.17	120.13	110.30
2	K	89	TYR	CB-CG-CD2	-5.17	117.90	121.00
2	H	206	ARG	CG-CD-NE	-5.17	100.94	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	186(A)	ASP	CA-CB-CG	-5.15	102.08	113.40
2	H	165	ARG	NE-CZ-NH1	-5.12	117.74	120.30
2	H	123	LEU	CB-CA-C	5.12	119.93	110.20
2	H	154	VAL	CA-CB-CG1	5.10	118.55	110.90
2	K	159	ASN	CA-CB-CG	5.09	124.59	113.40
2	K	61	GLU	CG-CD-OE2	-5.08	108.14	118.30
2	H	176	ILE	O-C-N	5.08	130.83	122.70
1	J	12	LEU	C-N-CA	5.08	134.39	121.70
3	R	418	GLY	N-CA-C	-5.05	100.47	113.10
2	K	102	ASP	CA-CB-CG	-5.04	102.32	113.40
3	R	421	CYS	CA-CB-SG	5.03	123.06	114.00

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	218	0	215	40	0
1	L	218	0	215	38	0
2	H	2007	0	1961	256	0
2	K	2007	0	1961	255	0
3	R	125	0	107	39	0
4	H	30	0	31	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	580	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 64.

All (580) 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	1.14
2:K:195:SER:HG	4:K:1:0G6:C2	1.56	1.12
2:K:233:ARG:HG2	2:K:233:ARG:HH11	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: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
2:K:201:MET:HE2	2:K:210:MET:HG3	1.41	0.98
1:L:14(A):LYS:CG	1:L:14(B):THR:HG23	1.93	0.98
2:K:205:ASN:C	2:K:205:ASN:HD22	1.66	0.97
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
3:R:415:LEU:HD13	3:R:422:THR:HB	1.46	0.94
2:K:107:LYS:CG	2:K:107:LYS:O	2.18	0.92
2:K:187:ARG:HG2	2:K:187:ARG:HH11	1.31	0.92
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	3:R:420:ILE:HD12	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:233:ARG:NH1	2:K:233:ARG:HG2	1.88	0.87
1:J:6:LEU:HD21	2:K:116:ASP:HB3	1.55	0.87
2:K:201:MET:HE3	2:K:210:MET:HG3	1.54	0.86
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:H:60:LEU:HD12	2:H:60(B):PRO:HD3	1.60	0.84
2:K:236:LYS:N	2:K:236:LYS:HD3	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:205:ASN:C	2:K:205:ASN:ND2	2.31	0.82
2:K:60(I):THR:CG2	2:K:61:GLU:H	1.93	0.81
2:H:213:VAL:O	2:H:213:VAL:HG12	1.79	0.81
2:H:76:TYR:CD2	3:R:422:THR:HG21	2.16	0.80
2:H:205:ASN:O	2:H:205:ASN:ND2	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:N	2:K:164:GLU:OE1	2.15	0.79
2:K:60:LEU:HD23	2:K:90:ILE:HD13	1.64	0.78
2:K:201:MET:CE	2:K:210:MET:CG	2.60	0.78
1:J:6:LEU:CD1	2:K:25:GLY:HA3	2.12	0.78
2:K:187:ARG:CG	2:K:187:ARG:HH11	1.91	0.78
2:H:126:ARG:NH1	2:H:127:GLU:CA	2.46	0.77
3:R:420:ILE:H	3:R:420:ILE:CD1	1.90	0.77
2:H:183:ALA:HB3	2:H:228:TYR:HE2	1.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:73:ARG:NH1	2:K:152:PRO:O	2.18	0.77
2:H:215:TRP:CE3	4:H:1:OG6:HD2	2.20	0.76
2:K:204(B):ASN:H	2:K:204(B):ASN:ND2	1.83	0.76
1:L:9:LYS:O	1:L:11:SER:N	2.20	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:H:46:LEU:HD21	2:H:112:VAL:HG11	1.69	0.75
2:H:188:GLY:O	2:H:189:ASP:HB2	1.85	0.74
2:H:32:MET:HE3	2:H:70:LYS:HD3	1.69	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: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:235:LYS:O	2:H:239:GLN:HG3	1.90	0.71
2:H:32:MET:HG3	2:H:141:TRP:CZ3	2.26	0.71
3:R:418:GLY:O	3:R:420:ILE:N	2.24	0.71
2:K:49:ASP:O	2:K:112:VAL:HG23	1.89	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:CD	2:K:236:LYS:N	2.53	0.70
1:L:10:LYS:NZ	1:L:10:LYS:HB3	2.06	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:N	2:K:204(B):ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:77(A):ARG:NH1	3:R:417:ASP:HB2	2.08	0.69
2:H:129(C):LEU:HD21	2:H:204:PRO:HD2	1.74	0.69
2:K:203:SER:OG	2:K:204(B):ASN:ND2	2.26	0.69
1:J:6:LEU:CD2	2:K:116:ASP:HB3	2.23	0.69
1:L:14(A):LYS:NZ	1:L:14(B):THR:OG1	2.26	0.69
2:K:23:GLU:O	2:K:26:MET:HB2	1.93	0.68
2:K:49:ASP:C	2:K:49:ASP:OD1	2.31	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:CZ	2:K:75:ARG:HB2	2.24	0.68
1:J:14(A):LYS:HG3	1:J:14(B):THR:HG22	1.75	0.68
2:H:46:LEU:CD1	2:H:48:SER:O	2.42	0.68
2:K:53:LEU:HD11	2:K:103:ILE:HD11	1.76	0.68
2:H:186(A):ASP:OD1	2:H:186(A):ASP:N	2.26	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
2:H:60(I):THR:C	2:H:62:ASN:H	1.94	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
2:K:195:SER:HG	4:K:1:OG6:H34	1.43	0.67
2:K:36:LYS:O	2:K:38:GLN:HG2	1.95	0.67
2:H:130:LEU:HD23	2:H:162:ILE:HD13	1.75	0.67
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:HB3	2:K:73:ARG:HH11	1.60	0.66
1:J:14(A):LYS:O	1:J:14(D):ARG:NH2	2.25	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:195:SER:CB	4:H:1:OG6:C2	2.75	0.65
2:H:60(A):TYR:C	2:H:60(C):PRO:HD2	2.17	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:K:201:MET:HE3	2:K:210:MET:CG	2.24	0.65
2:K:31:VAL:HG22	2:K:68:ILE:HG23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:182:CYS:HA	2:H:226:GLY:O	1.97	0.65
2:K:142:GLY:O	2:K:152:PRO:CD	2.45	0.65
2:H:105:LEU:HD13	2:H:241:VAL:CG2	2.26	0.65
2:H:105:LEU:HD13	2:H:241:VAL:HG22	1.78	0.65
2:H:51:TRP:NE1	2:H:242:ILE:HG23	2.11	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:HD3	1:J:14(D):ARG:H	1.62	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:77(A):ARG:HH12	3:R:417:ASP:HB2	1.62	0.64
2:K:70:LYS:NZ	2:K:77:GLU:OE1	2.31	0.64
2:H:60(B):PRO:HG2	2:H:96:TRP:CD2	2.33	0.64
2:H:16:ILE:HG12	2:H:194:ASP:OD2	1.97	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:H:134:TYR:HD1	2:H:134:TYR:N	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
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
2:H:172:THR:OG1	2:H:173:ARG:N	2.32	0.63
2:H:41:LEU:HD22	2:H:64:LEU:HD12	1.77	0.62
2:K:195:SER:HG	4:K:1:OG6:H33	1.46	0.62
1:L:9:LYS:C	1:L:11:SER:N	2.51	0.62
2:H:68:ILE:CG2	2:H:118:ILE:HG23	2.30	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:H:199:PHE:HE1	2:H:201:MET:HE2	1.64	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
2:H:81:LYS:NZ	2:H:113:ALA:HB3	2.14	0.62
1:L:6:LEU:HD23	1:L:10:LYS:HD2	1.82	0.62
2:K:208:TYR:HB2	2:K:210:MET:HE2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:59:LEU:HD11	2:K:106:MET:HE3	1.82	0.61
1:J:10:LYS:NZ	5:J:710:HOH:O	2.34	0.61
2:K:165:ARG:C	2:K:169:LYS:HE3	2.21	0.61
2:H:32:MET:HE3	2:H:70:LYS:CD	2.29	0.61
2:H:85:LEU:HD13	2:H:88:ILE:HD11	1.82	0.61
2:H:60(I):THR:C	2:H:62:ASN:N	2.54	0.61
2:K:195:SER:HA	2:K:213:VAL:HG12	1.83	0.61
2:H:195:SER:CB	4:H:1:0G6:C3	2.78	0.61
2:K:139:THR:HB	2:K:155:LEU:HD11	1.83	0.60
2:H:49:ASP:O	2:H:111:PRO:HA	2.01	0.60
2:K:99:LEU:HD11	4:K:1:0G6:HA1	1.82	0.60
2:H:79:ILE:HG22	2:H:80:GLU:N	2.15	0.60
2:H:26:MET:O	2:H:26:MET:HG2	2.02	0.60
1:L:10:LYS:HZ3	1:L:10:LYS:HB3	1.65	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
2:H:67:ARG:CD	2:H:80:GLU:OE2	2.50	0.60
2:K:53:LEU:HD11	2:K:103:ILE:CD1	2.32	0.60
1:L:7:PHE:O	1:L:11:SER:N	2.35	0.60
2:K:23:GLU:HA	5:K:727:HOH:O	2.01	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:195:SER:OG	4:H:1:0G6:C3	2.48	0.59
2:K:103:ILE:HG21	2:K:234:LEU:HD13	1.82	0.59
2:K:60(I):THR:C	2:K:62:ASN:H	2.05	0.59
2:H:22:ALA:CB	2:H:155:LEU:HB3	2.33	0.59
4:H:1:0G6:CD1	4:H:1:0G6:HD3	2.33	0.58
2:H:174:ILE:HD12	2:H:215:TRP:CZ3	2.38	0.58
2:H:134:TYR:N	2:H:134:TYR:CD1	2.71	0.58
2:H:164:GLU:O	2:H:167:VAL:HB	2.03	0.58
2:H:231:VAL:HG13	2:H:232:PHE:N	2.18	0.58
2:K:125:ASP:CG	2:K:128:THR:HB	2.24	0.58
1:J:7:PHE:HB3	1:J:12:LEU:O	2.03	0.58
2:H:114:PHE:HB3	2:H:118:ILE:O	2.03	0.58
2:K:182:CYS:HA	2:K:226:GLY:O	2.03	0.58
2:H:153:SER:O	2:H:154:VAL:HG23	2.02	0.58
3:R:418:GLY:O	3:R:420:ILE:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:236:LYS:H	2:K:236:LYS:HD3	1.65	0.58
2:H:68:ILE:HG22	2:H:118:ILE:HG23	1.86	0.57
2:K:165:ARG:O	2:K:169:LYS:HG3	2.04	0.57
2:K:31:VAL:HB	2:K:44:ALA:HB3	1.87	0.57
2:H:184(A):TYR:HB3	2:H:186(B):GLU:HB2	1.86	0.57
2:H:60(I):THR:N	2:H:63:ASP:OD2	2.36	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:HG3	2:K:39:GLU:O	2.05	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
2:H:98:ASN:ND2	2:H:175:ARG:O	2.30	0.56
1:L:4:ARG:NH2	1:L:14:ASP:OD2	2.38	0.56
2:H:60:LEU:CD1	2:H:60(B):PRO:HD3	2.32	0.56
1:L:14(G):LEU:HD11	2:H:202:LYS:HD3	1.87	0.56
1:L:9:LYS:C	1:L:11:SER:H	2.09	0.56
2:K:185:LYS:C	2:K:186(A):ASP:H	2.09	0.56
2:H:42:CYS:HB3	2:H:195:SER:O	2.04	0.56
1:L:7:PHE:CE1	2:H:26:MET:HA	2.40	0.56
1:L:6:LEU:HA	1:L:10:LYS:HD3	1.88	0.56
2:K:127:GLU:HA	2:K:129(A):ALA:HB3	1.87	0.56
2:K:31:VAL:CG1	2:K:66:VAL:HG13	2.35	0.56
2:K:88:ILE:HG12	2:K:106:MET:HB3	1.88	0.56
2:H:189:ASP:OD1	2:H:190:ALA:N	2.39	0.56
4:K:1:0G6:HD3	4:K:1:0G6:CD1	2.36	0.56
2:K:60(B):PRO:HG2	2:K:96:TRP:CE3	2.41	0.56
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:H:145:LYS:HB2	2:H:148:TRP:CB	2.36	0.55
2:K:29:TRP:CG	2:K:121:VAL:HB	2.41	0.55
2:H:60(B):PRO:HG2	2:H:96:TRP:CE3	2.41	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:O	2:H:57:HIS:CD2	2.59	0.55
2:H:145:LYS:HD3	2:H:148:TRP:CB	2.37	0.55
1:J:6:LEU:HD21	2:K:116:ASP:CB	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:88:ILE:HG12	2:H:106:MET:CB	2.37	0.54
2:H:125:ASP:O	2:H:126:ARG:C	2.45	0.54
2:H:166:PRO:O	2:H:167:VAL:C	2.46	0.54
2:K:168:CYS:C	2:K:171:SER:HB3	2.27	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:H:32:MET:HE3	2:H:70:LYS:CE	2.37	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:H:32:MET:CE	2:H:70:LYS:HD3	2.35	0.54
2:K:195:SER:CB	4:K:1:OG6:H33	2.37	0.54
2:H:125:ASP:C	2:H:127:GLU:N	2.57	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
1:L:14(I):SER:OG	2:H:134:TYR:HA	2.08	0.54
2:H:215:TRP:HA	4:H:1:OG6:HB32	1.90	0.54
2:H:125:ASP:N	2:H:125:ASP:OD1	2.40	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:126:ARG:HH11	2:H:127:GLU:CA	2.19	0.53
2:H:54:THR:HG23	2:H:55:ALA:N	2.24	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
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
3:R:420:ILE:N	3:R:420:ILE:CD1	2.53	0.53
2:K:145:LYS:O	2:K:146:GLU:C	2.48	0.53
3:R:415:LEU:HD13	3:R:422:THR:CB	2.30	0.53
2:K:60(A):TYR:CZ	4:K:1:OG6:HG2	2.44	0.53
2:H:89:TYR:N	2:H:89:TYR:CD1	2.77	0.53
2:K:212:ILE:HB	2:K:229:THR:HB	1.90	0.53
2:K:235:LYS:O	2:K:235:LYS:HG2	2.09	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
3:R:416:ASP:CG	3:R:416:ASP:O	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:56:ALA:HB2	2:K:103:ILE:O	2.10	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
1:J:9:LYS:C	1:J:11:SER:H	2.11	0.51
2:H:203:SER:O	2:H:205:ASN:HA	2.11	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
3:R:410:PRO:C	3:R:412:GLY:H	2.12	0.51
2:K:203:SER:O	2:K:205:ASN:HA	2.10	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:70:LYS:NZ	2:K:72:SER:O	2.36	0.50
1:L:9:LYS:O	1:L:10:LYS:C	2.49	0.50
1:J:14(J):TYR:HD1	2:K:134:TYR:CD2	2.29	0.50
2:H:81:LYS:HZ2	2:H:113:ALA:HB3	1.76	0.50
2:K:18:GLU:HB2	2:K:188:GLY:HA2	1.93	0.50
2:K:208:TYR:CB	2:K:210:MET:CE	2.89	0.50
2:K:17:VAL:HG11	2:K:221:ASP:HB3	1.93	0.50
2:K:155:LEU:HD12	2:K:156:GLN:H	1.77	0.50
2:K:36(A):SER:OG	2:K:36(A):SER:O	2.30	0.50
1:J:14(A):LYS:NZ	1:J:14(B):THR:CG2	2.75	0.50
2:K:208:TYR:HB2	2:K:210:MET:CE	2.42	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
1:J:1:CYS:O	2:K:122:CYS:SG	2.70	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
2:H:80:GLU:CG	2:H:81:LYS:N	2.71	0.49
3:R:415:LEU:CD1	3:R:422:THR:HB	2.31	0.49
2:K:59:LEU:HD11	2:K:106:MET:CE	2.41	0.49
2:K:164:GLU:O	2:K:165:ARG:C	2.51	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
1:L:10:LYS:NZ	1:L:10:LYS:CB	2.70	0.49
2:K:242:ILE:CG2	2:K:242:ILE:O	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:94:TYR:HB2	2:H:101:ARG:O	2.13	0.49
2:H:86:GLU:HB2	2:H:109:LYS:HA	1.95	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:K:75:ARG:NH2	2:K:75:ARG:HB2	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:213:VAL:CG1	2:H:213:VAL:O	2.47	0.48
3:R:416:ASP:O	3:R:416:ASP:OD1	2.31	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
2:H:165:ARG:HB2	2:H:166:PRO:HD3	1.94	0.48
2:H:71:HIS:O	2:H:154:VAL:HA	2.14	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: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
2:H:141:TRP:HA	2:H:152:PRO:HG2	1.95	0.48
1:J:14(G):LEU:C	1:J:14(I):SER:N	2.65	0.48
2:K:26:MET:HE2	2:K:137:ARG:NH1	2.29	0.48
2:K:31:VAL:HG13	2:K:66:VAL:HG13	1.95	0.48
2:H:146:GLU:HA	2:H:220:CYS:HB2	1.95	0.48
2:H:28:PRO:HB2	2:H:119:HIS:HB3	1.95	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
1:L:14(D):ARG:HG2	1:L:14(H):GLU:OE2	2.14	0.48
2:K:60(I):THR:CG2	2:K:61:GLU:N	2.54	0.48
2:K:35:ARG:NH1	2:K:37:PRO:HD2	2.29	0.48
2:K:130:LEU:HD22	2:K:162:ILE:CD1	2.44	0.47
2:H:68:ILE:HG21	2:H:118:ILE:HG23	1.96	0.47
1:J:14(A):LYS:HZ3	1:J:14(B):THR:HG22	1.79	0.47
2:H:38:GLN:HE22	3:R:414:ILE:H	1.62	0.47
1:L:7:PHE:CE2	1:L:14:ASP:HB3	2.49	0.47
2:H:190:ALA:O	2:H:191:CYS:HB2	2.14	0.47
2:K:208:TYR:CB	2:K:210:MET:HE1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:91:HIS:CB	2:K:103:ILE:HG23	2.32	0.47
2:K:71:HIS:NE2	2:K:154:VAL:CG1	2.78	0.47
2:H:151:GLN:HA	2:H:152:PRO:HD3	1.80	0.47
2:K:98:ASN:ND2	2:K:175:ARG:HB3	2.30	0.47
1:J:5:PRO:HA	1:J:9:LYS:HD2	1.95	0.47
2:K:240:LYS:C	2:K:242:ILE:N	2.67	0.47
2:H:186:PRO:HD3	2:H:223:GLY:HA2	1.97	0.47
2:H:16:ILE:HG21	2:H:158:VAL:HB	1.96	0.47
2:H:34:PHE:CG	3:R:413:TYR:OH	2.66	0.47
2:H:201:MET:CE	2:H:210:MET:HG3	2.45	0.47
2:K:91:HIS:HB2	2:K:103:ILE:CG2	2.31	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
1:L:4:ARG:NH1	2:H:207:TRP:NE1	2.60	0.47
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.78	0.47
2:K:185:LYS:H	2:K:186(B):GLU:HG3	1.79	0.47
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
1:L:14(B):THR:O	1:L:14(E):GLU:HB3	2.15	0.46
2:K:60(A):TYR:C	2:K:60(C):PRO:HD2	2.35	0.46
2:K:60(I):THR:C	2:K:62:ASN:N	2.69	0.46
2:K:110:LYS:HA	2:K:111:PRO:HD3	1.84	0.46
2:H:19:GLY:HA2	2:H:158:VAL:HG23	1.97	0.46
2:H:36(A):SER:HA	2:H:37:PRO:C	2.35	0.46
2:K:17:VAL:HG11	2:K:221:ASP:CB	2.45	0.46
2:K:36(A):SER:HA	2:K:37:PRO:C	2.36	0.46
2:K:86:GLU:HA	2:K:109:LYS:HE3	1.98	0.46
1:L:14(J):TYR:CD2	2:H:204:PRO:HG3	2.51	0.46
2:K:167:VAL:O	2:K:171:SER:CB	2.64	0.46
2:K:52:VAL:O	2:K:105:LEU:HD23	2.15	0.46
2:K:49:ASP:O	2:K:111:PRO:HA	2.15	0.46
3:R:422:THR:HG23	3:R:424:ILE:HG23	1.98	0.46
2:K:124:PRO:HD3	2:K:209:GLN:O	2.16	0.46
2:H:236:LYS:N	2:H:236:LYS:HD3	2.30	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
1:J:4:ARG:HD3	1:J:8:GLU:OE1	2.15	0.45
2:H:68:ILE:HB	2:H:118:ILE:HD13	1.97	0.45
2:H:199:PHE:HE1	2:H:201:MET:CE	2.28	0.45
2:H:105:LEU:HD13	2:H:241:VAL:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:174:ILE:HG22	2:H:175:ARG:N	2.31	0.45
2:K:71:HIS:NE2	2:K:154:VAL:HG11	2.32	0.45
2:H:184(A):TYR:CE2	2:H:186(D):LYS:HB2	2.51	0.45
2:H:17:VAL:HG13	2:H:144:LEU:O	2.17	0.45
2:H:192:GLU:OE2	5:H:915:HOH:O	2.21	0.45
2:H:40:LEU:HG	2:H:41:LEU:N	2.31	0.45
2:K:213:VAL:HG22	2:K:228:TYR:HE1	1.82	0.45
2:K:86:GLU:CB	2:K:109:LYS:HG2	2.47	0.45
1:J:10:LYS:HB3	1:J:10:LYS:HE2	1.69	0.45
2:H:109:LYS:C	2:H:110:LYS:HG2	2.35	0.45
2:H:51:TRP:HE3	2:H:105:LEU:HD22	1.80	0.45
2:H:30:GLN:OE1	2:H:198:PRO:HD2	2.15	0.45
2:H:67:ARG:NH2	2:H:70:LYS:HE2	2.31	0.45
2:K:91:HIS:ND1	2:K:92:PRO:HD2	2.32	0.45
2:K:85:LEU:HD23	2:K:106:MET:HB2	1.98	0.45
2:H:205:ASN:HD22	2:H:205:ASN:C	2.20	0.45
1:L:10:LYS:HZ2	1:L:10:LYS:CB	2.30	0.45
2:H:215:TRP:CD2	4:H:1:OG6:HD2	2.50	0.45
2:H:126:ARG:HD3	2:H:127:GLU:OE1	2.16	0.45
2:H:231:VAL:CG1	2:H:232:PHE:N	2.79	0.45
2:H:51:TRP:CD1	2:H:242:ILE:HD13	2.51	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
2:K:98:ASN:N	2:K:98:ASN:OD1	2.50	0.44
1:J:14(J):TYR:HE2	2:K:202:LYS:O	1.99	0.44
3:R:418:GLY:C	3:R:420:ILE:N	2.70	0.44
2:H:29:TRP:CD2	2:H:121:VAL:HB	2.52	0.44
2:H:125:ASP:O	2:H:127:GLU: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:91:HIS:CE1	2:H:93:ARG:H	2.35	0.44
2:H:64:LEU:N	2:H:64:LEU:HD22	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:17:VAL:HG21	2:H:220:CYS:HB3	2.00	0.44
2:H:217:GLU:OE1	2:H:224:LYS:HE2	2.18	0.44
2:K:99:LEU:CD1	2:K:215:TRP:HB3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:70:LYS:HE2	2:K:80:GLU:OE2	2.18	0.44
2:K:204(A):PHE:N	2:K:204(A):PHE:CD1	2.84	0.44
2:H:141:TRP:CE2	2:H:155:LEU:HD13	2.52	0.44
2:H:76:TYR:CZ	3:R:424:ILE:CG2	2.99	0.44
2:H:184(A):TYR:CE2	2:H:186(D):LYS:CB	3.01	0.44
1:J:14(G):LEU:C	1:J:14(I):SER:H	2.16	0.43
2:K:144:LEU:HA	2:K:144:LEU:HD12	1.83	0.43
2:K:31:VAL:CG1	2:K:44:ALA:HB3	2.48	0.43
2:K:208:TYR:HB3	2:K:210:MET:HE1	1.99	0.43
2:H:201:MET:HE3	2:H:201:MET:HB2	1.74	0.43
1:J:14(D):ARG:N	1:J:14(D):ARG:HD3	2.31	0.43
2:K:82:ILE:CD1	3:R:420:ILE:HG12	2.48	0.43
2:H:61:GLU:HG2	2:H:62:ASN:OD1	2.18	0.43
2:K:235:LYS:HE2	2:K:239:GLN:HE21	1.82	0.43
2:K:95:ASN:ND2	2:K:97(A):GLU:HB3	2.31	0.43
2:H:96:TRP:CH2	2:H:97:ARG:NH2	2.85	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
2:H:96:TRP:HZ2	2:H:97:ARG:NH2	2.13	0.43
2:H:157:VAL:O	2:H:157:VAL:HG23	2.19	0.43
1:L:14(J):TYR:OH	2:H:201:MET:HG2	2.18	0.43
1:L:6:LEU:HD23	1:L:10:LYS:CD	2.47	0.43
2:K:141:TRP:O	2:K:151:GLN:OE1	2.37	0.43
1:J:9:LYS:C	1:J:11:SER:N	2.70	0.43
2:K:86:GLU:HB2	2:K:109:LYS:HG2	2.00	0.43
2:K:31:VAL:CB	2:K:44:ALA:HB3	2.48	0.43
2:H:165:ARG:CB	2:H:166:PRO:CD	2.97	0.43
2:H:107:LYS:HG2	2:H:108:LEU:O	2.19	0.43
2:H:88:ILE:HG12	2:H:106:MET:HB3	2.00	0.42
2:H:99:LEU:HD11	4:H:1:0G6:HB21	2.01	0.42
2:H:98:ASN:HD22	2:H:175:ARG:HB3	1.84	0.42
2:K:61:GLU:OE1	2:K:87:LYS:HA	2.19	0.42
2:K:33:LEU:HD11	2:K:106:MET:HE3	2.01	0.42
1:L:1:CYS:O	2:H:206:ARG:HD3	2.19	0.42
2:H:200:VAL:HG12	2:H:208:TYR:O	2.20	0.42
2:H:32:MET:HE3	2:H:67:ARG:NH2	2.35	0.42
2:K:148:TRP:O	2:K:149:THR:C	2.56	0.42
2:H:144:LEU:HA	2:H:144:LEU:HD23	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:152:PRO:HB3	2:K:156:GLN:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:147:THR:HG23	2:K:147:THR:O	2.20	0.42
1:L:3:LEU:HG	2:H:206:ARG:HG2	2.02	0.42
1:J:3:LEU:HA	1:J:3:LEU:HD23	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:155:LEU:HD12	2:H:155:LEU:HA	1.46	0.42
2:H:82:ILE:HD13	3:R:413:TYR:CE2	2.55	0.42
2:K:129:ALA:O	2:K:130:LEU:HB2	2.20	0.42
2:H:70:LYS:NZ	2:H:75:ARG:O	2.38	0.41
2:H:235:LYS:HE2	2:H:239:GLN:HE21	1.85	0.41
1:L:6:LEU:HG	2:H:116:ASP:HB3	2.02	0.41
2:K:148:TRP:CB	2:K:150:GLY:N	2.83	0.41
2:K:143:ASN:HD21	2:K:149:THR:CA	2.33	0.41
2:H:60(G):ASN:O	5:H:901:HOH:O	2.21	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:H:130:LEU:HA	2:H:130:LEU:HD23	1.89	0.41
2:K:60(B):PRO:O	2:K:60(C):PRO:C	2.57	0.41
2:K:168:CYS:O	2:K:171:SER:CB	2.56	0.41
2:K:34:PHE:CE2	2:K:38:GLN:HB3	2.55	0.41
2:H:34:PHE:CD2	3:R:413:TYR:OH	2.73	0.41
2:K:57:HIS:CE1	2:K:214:SER:O	2.74	0.41
2:H:232:PHE:HA	2:H:235:LYS:HB2	2.02	0.41
2:H:145:LYS:O	2:H:146:GLU:C	2.58	0.41
2:H:125:ASP:C	2:H:127:GLU:H	2.22	0.41
2:H:185:LYS:HB3	2:H:186(A):ASP:OD1	2.21	0.41
2:H:165:ARG:CB	2:H:166:PRO:HD3	2.51	0.41
2:H:225:TYR:N	2:H:225:TYR:CD1	2.89	0.41
2:H:216:GLY:O	4:H:1:OG6:N	2.54	0.41
2:H:98:ASN:N	2:H:98:ASN:OD1	2.53	0.41
2:K:73:ARG:HB3	2:K:73:ARG:NH1	2.30	0.41
2:K:195:SER:HA	2:K:213:VAL:O	2.20	0.41
2:K:115:SER:C	2:K:117:TYR:H	2.19	0.41
2:H:76:TYR:CE1	2:H:82:ILE:HD11	2.55	0.41
2:K:215:TRP:CE3	4:K:1:OG6:HD2	2.56	0.41
2:K:152:PRO:CB	2:K:156:GLN:HG2	2.51	0.41
2:K:151:GLN:HA	2:K:152:PRO:HD3	1.94	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:H:186:PRO:HG3	2:H:223:GLY:HA3	2.03	0.41
2:H:114:PHE:CZ	2:H:120:PRO:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:12:LEU:HD12	5:L:910:HOH:O	2.20	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:97(A):GLU:OE1	2:K:175:ARG:HD3	2.21	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:171:SER:O	2:H:224:LYS:HE3	2.20	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:HG2	2:H:126:ARG:O	2.21	0.40
2:K:41:LEU:HD23	2:K:64:LEU:CD1	2.42	0.40
2:K:28:PRO:HB2	2:K:119:HIS:HB3	2.03	0.40
2:H:87:LYS:HB3	2:H:89:TYR:HE1	1.85	0.40
1:J:14(G):LEU:HA	1:J:14(G):LEU:HD23	1.66	0.40
2:H:127:GLU:O	2:H:129(A):ALA:HB3	2.22	0.40
1:J:5:PRO:C	1:J:7:PHE:N	2.75	0.40
2:K:59:LEU:HD23	2:K:88:ILE:CG2	2.51	0.40
1:J:1:CYS:SG	1:J:1:CYS:O	2.80	0.40
2:H:60(I):THR:O	2:H:62:ASN:N	2.54	0.40
2:H:49:ASP:N	2:H:49:ASP:OD1	2.37	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	25/27 (93%)	17 (68%)	7 (28%)	1 (4%)	4	21
1	L	25/27 (93%)	17 (68%)	5 (20%)	3 (12%)	0	2
2	H	247/259 (95%)	209 (85%)	29 (12%)	9 (4%)	4	24
2	K	247/259 (95%)	212 (86%)	30 (12%)	5 (2%)	9	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	R	15/19 (79%)	8 (53%)	4 (27%)	3 (20%)	0	0
All	All	559/591 (95%)	463 (83%)	75 (13%)	21 (4%)	4	22

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
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%)	21 (88%)	3 (12%)	6	24
1	L	24/25 (96%)	18 (75%)	6 (25%)	1	3
2	H	214/225 (95%)	183 (86%)	31 (14%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	214/225 (95%)	174 (81%)	40 (19%)	2	10
3	R	13/17 (76%)	7 (54%)	6 (46%)	0	0
All	All	489/517 (95%)	403 (82%)	86 (18%)	2	12

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	10	LYS
1	L	14(A)	LYS
1	L	14(C)	GLU
1	L	14(D)	ARG
1	L	14(F)	LEU
1	L	14(I)	SER
2	H	18	GLU
2	H	50	ARG
2	H	54	THR
2	H	59	LEU
2	H	60(I)	THR
2	H	62	ASN
2	H	64	LEU
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	125	ASP
2	H	126	ARG
2	H	127	GLU
2	H	128	THR
2	H	151	GLN
2	H	159	ASN
2	H	160	LEU
2	H	165	ARG
2	H	172	THR
2	H	176	ILE
2	H	181	PHE
2	H	182	CYS
2	H	185	LYS
2	H	199	PHE
2	H	200	VAL

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Mol	Chain	Res	Type
2	H	205	ASN
2	H	206	ARG
2	H	224	LYS
1	J	10	LYS
1	J	14(B)	THR
1	J	14(D)	ARG
2	K	16	ILE
2	K	18	GLU
2	K	20	SER
2	K	27	SER
2	K	36(A)	SER
2	K	48	SER
2	K	52	VAL
2	K	54	THR
2	K	61	GLU
2	K	63	ASP
2	K	64	LEU
2	K	68	ILE
2	K	75	ARG
2	K	81	LYS
2	K	83	SER
2	K	85	LEU
2	K	86	GLU
2	K	103	ILE
2	K	106	MET
2	K	107	LYS
2	K	125	ASP
2	K	126	ARG
2	K	127	GLU
2	K	128	THR
2	K	129(B)	SER
2	K	130	LEU
2	K	159	ASN
2	K	171	SER
2	K	182	CYS
2	K	186(A)	ASP
2	K	187	ARG
2	K	192	GLU
2	K	194	ASP
2	K	195	SER
2	K	204(B)	ASN
2	K	205	ASN

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Mol	Chain	Res	Type
2	K	231	VAL
2	K	233	ARG
2	K	236	LYS
2	K	241	VAL
3	R	413	TYR
3	R	415	LEU
3	R	416	ASP
3	R	417	ASP
3	R	419	PHE
3	R	420	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	38	GLN
2	H	78	ASN
2	H	143	ASN
2	H	205	ASN
2	H	239	GLN
2	K	38	GLN
2	K	71	HIS
2	K	143	ASN
2	K	204(B)	ASN
2	K	205	ASN
2	K	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 carbohydrates in this entry.

5.6 Ligand geometry

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	H	1	2	27,31,32	1.10	3 (11%)	35,41,42	3.10	14 (40%)
4	0G6	K	1	2	27,31,32	0.92	1 (3%)	35,41,42	1.89	9 (25%)

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	H	1	2	-	0/29/41/43	0/2/2/2
4	0G6	K	1	2	-	0/29/41/43	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	-2.64	1.27	1.34
4	H	1	0G6	CA2-N2	-2.43	1.42	1.46
4	H	1	0G6	CB1-CA1	-2.20	1.48	1.53
4	K	1	0G6	C3-C2	2.04	1.56	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	0G6	C1-CA1-N1	-3.92	102.62	112.59
4	H	1	0G6	O1-C1-CA1	-3.06	113.48	120.51
4	K	1	0G6	O-C-CA	-2.66	114.49	119.58
4	K	1	0G6	O2-C2-C3	-2.45	102.51	109.61
4	K	1	0G6	C1-CA1-N1	-2.44	106.38	112.59
4	H	1	0G6	CA-C-N1	-2.08	115.05	118.85
4	H	1	0G6	CG1-CD-N1	2.09	106.52	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	0G6	CB-CA-C	2.16	113.64	108.80
4	H	1	0G6	CG-CB-CA	2.20	119.49	114.31
4	K	1	0G6	CB1-CA1-N1	2.23	106.17	102.99
4	K	1	0G6	CA1-C1-N2	2.23	121.67	116.64
4	H	1	0G6	O1-C1-N2	2.53	127.89	122.93
4	H	1	0G6	O-C-N1	2.62	125.91	121.41
4	H	1	0G6	CB1-CA1-N1	3.06	107.36	102.99
4	H	1	0G6	O2-C2-CA2	3.14	115.64	108.58
4	H	1	0G6	C2-CA2-N2	3.36	116.41	110.11
4	K	1	0G6	CG2-CB2-CA2	3.42	121.31	114.10
4	K	1	0G6	O-C-N1	3.50	127.42	121.41
4	H	1	0G6	CB1-CA1-C1	3.53	117.75	111.26
4	K	1	0G6	CA2-N2-C1	4.20	130.94	123.13
4	H	1	0G6	CB2-CA2-N2	4.67	117.05	110.41
4	K	1	0G6	CB2-CA2-N2	4.95	117.46	110.41
4	H	1	0G6	CA2-N2-C1	13.89	148.95	123.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 22 short contacts:

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.