



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:40 am GMT

PDB ID : 3JA8  
EMDB ID: : EMD-6338  
Title : Cryo-EM structure of the MCM2-7 double hexamer  
Authors : Li, N.; Zhai, Y.; Zhang, Y.; Li, W.; Yang, M.; Lei, J.; Tye, B.K.; Gao, N.  
Deposited on : 2015-05-09  
Resolution : 3.80 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

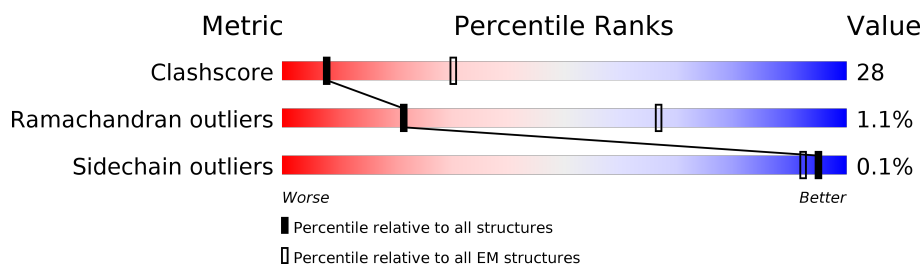
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	2	868	
2	3	971	
3	4	933	
4	5	775	
5	6	1017	
6	7	845	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	ADP	6	2001	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 29838 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Minichromosome Maintenance 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	603	Total	C	N	O	S	0	0
			4714	2974	842	881	17		

- Molecule 2 is a protein called Minichromosome Maintenance 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	605	Total	C	N	O	S	0	0
			4745	2990	846	896	13		

- Molecule 3 is a protein called Minichromosome Maintenance 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	640	Total	C	N	O	S	0	0
			5081	3194	879	981	27		

- Molecule 4 is a protein called Minichromosome Maintenance 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	633	Total	C	N	O	S	0	0
			4962	3112	855	971	24		

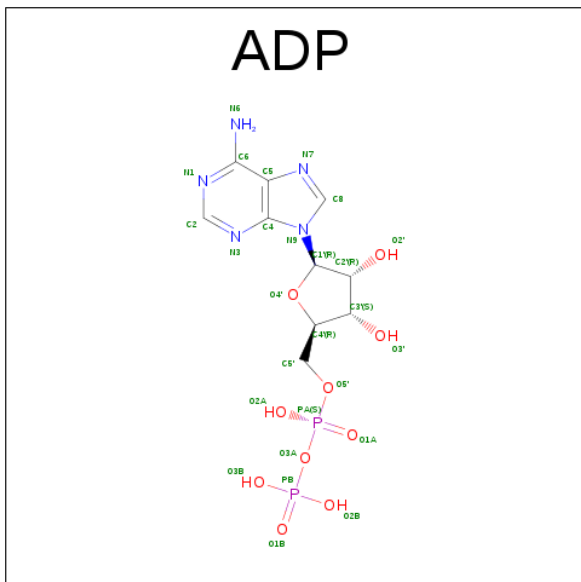
- Molecule 5 is a protein called Minichromosome Maintenance 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	616	Total	C	N	O	S	0	0
			4742	2985	841	896	20		

- Molecule 6 is a protein called Minichromosome Maintenance 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	689	Total	C	N	O	S	0	0
			5432	3419	940	1042	31		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).

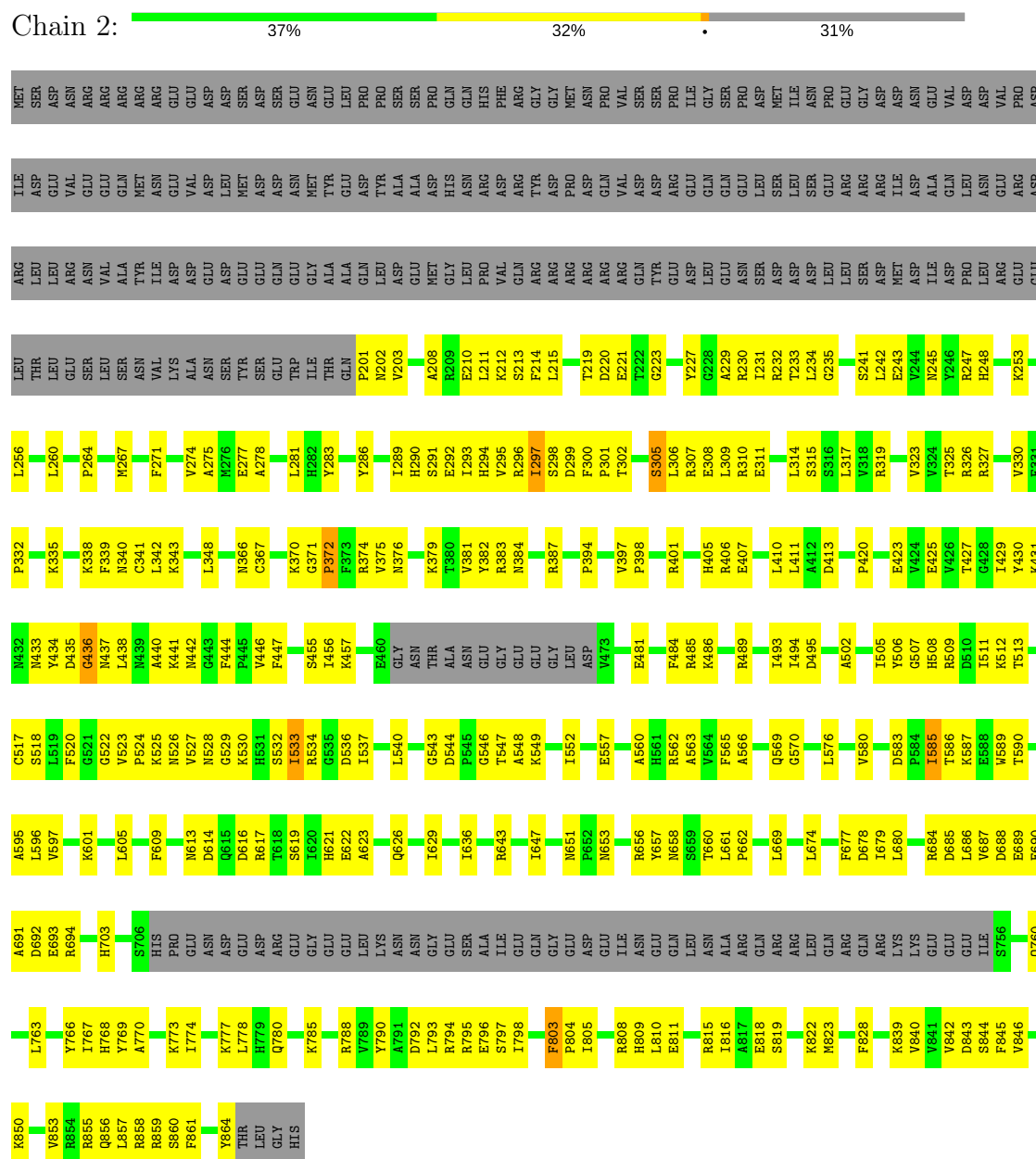


Mol	Chain	Residues	Atoms					AltConf
7	2	1	Total 27	C 10	N 5	O 10	P 2	0
7	3	1	Total 27	C 10	N 5	O 10	P 2	0
7	4	1	Total 27	C 10	N 5	O 10	P 2	0
7	5	1	Total 27	C 10	N 5	O 10	P 2	0
7	6	1	Total 27	C 10	N 5	O 10	P 2	0
7	7	1	Total 27	C 10	N 5	O 10	P 2	0

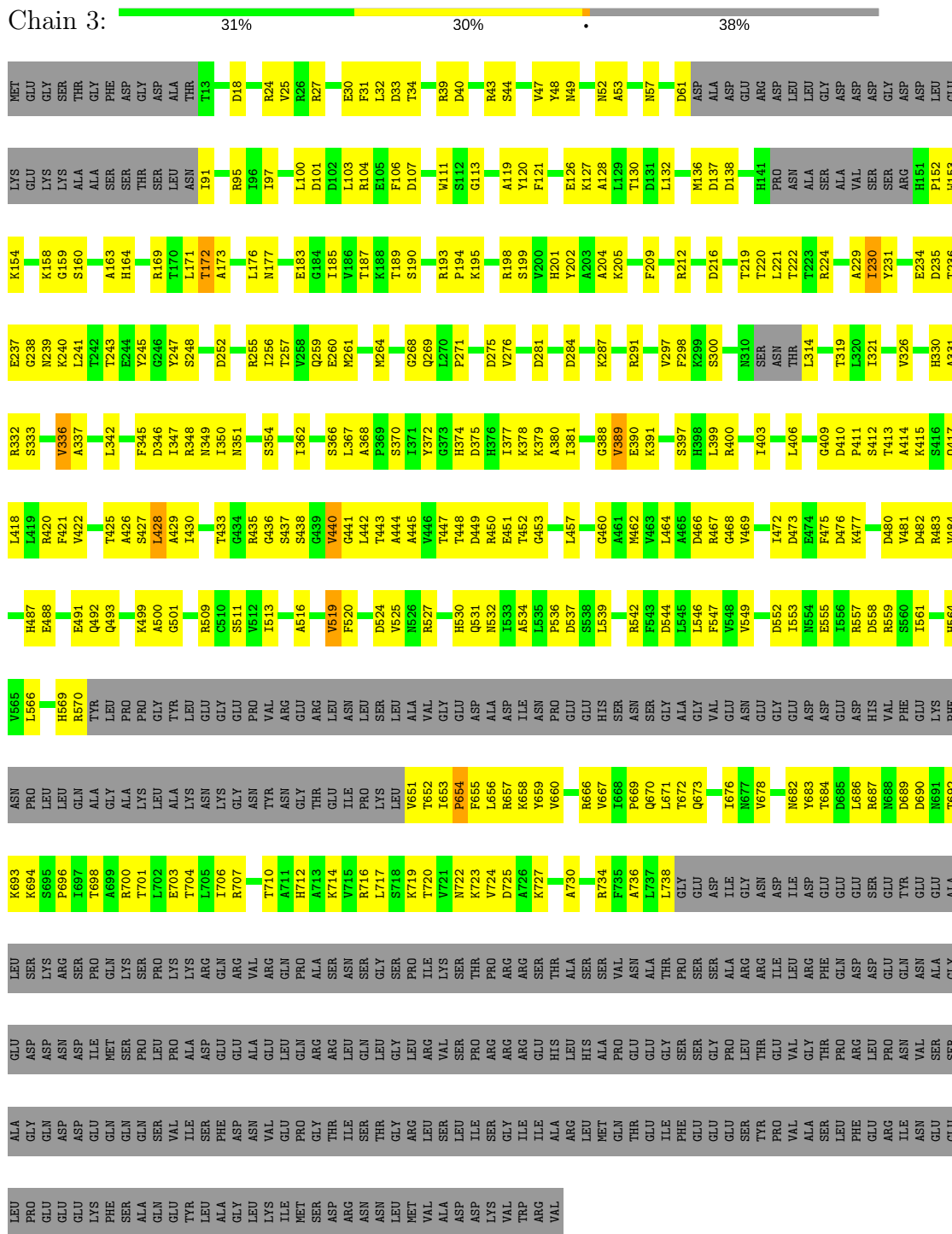
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

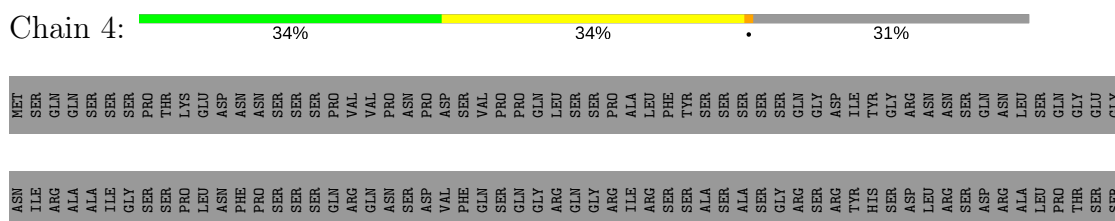
- Molecule 1: Minichromosome Maintenance 2



- Molecule 2: Minichromosome Maintenance 3



● Molecule 3: Minichromosome Maintenance 4



SER	M184	T254	V392	G409	T478	R559	V648	P733	M811	ALA
SER	M185	L257	L333	Q410	E482	G560	M649	S737	SER	SER
LEU	V186	L263	L334	T411	E483	D561	E650	S737	ASP	ASP
GLY	S186	L262	P337	T412	Q483	I562	Q651	L742	L813	ASP
ARG	I187	Q260	P340	H413	E484	N563	S655	P743	V817	MET
ASN	Q188	L261	D341	S414	L485	I564	I656	F746	E818	SER
GLY	E189	L262	M342	T415	N488	L565	I657	L747	L819	PHE
GLN	C190	N263	K344	S416	K489	L566	A657	L747	E820	ASN
ASN	T191	N263	K344	L417	C567	L567	K658	L747	E821	ASN
VAL	N196	Y264	K344	C418	D491	G568	I662	L751	Q822	LEU
HIS	F197	Y265	A345	V419	H492	D569	I662	L751	Q823	ILE
MET	K202	Q266	F346	Y420	N493	P570	N666	L758	Q827	LYS
ARG	Y203	Q267	F347	Y421	E494	S571	A667	H759	R827	ILE
ASN	R206	V268	K348	E422	E497	T572	R668	I761	R830	ASN
ASP	L271	I269	C349	R428	V498	S573	I669	I762	S831	ASN
ILE	L209	L276	C352	D431	T502	K574	A675	I763	A832	HIS
THR	D210	L276	D353	R432	D503	S575	I676	E764	I833	GLN
SER	E211	L284	H354	R433	D503	L578	I677	K767	Y836	ASP
ASP	R212	D280	T355	E434	Q504	T585	I678	K767	A837	ARG
LEU	GLU	M281	M356	V435	D505	P586	G679	E769	T838	VAL
SER	PHE	Y281	A357	T436	L506	R587	G680	L770	ASP	GLU
PRO	ILE	I284	I360	G437	I509	S592	R681	L771	LYS	SER
ARG	ASN	D290	D361	F439	R510	G593	I682	R772	THR	ASP
THR	THR	Y291	R362	L442	V512	K594	V688	I774	GLY	ILE
VAL	D221	L293	E367	R445	R515	A598	N691	M777	GLY	GLU
ASP	E222	E297	R370	R446	E516	V599	I692	R778	ASP	ALA
PHE	E223	T298	C371	R446	D517	G600	D693	K779	MET	LEU
THR	L224	K299	E372	S448	L518	L602	L694	GLY	LEU	LEU
ARG	Y225	F300	R373	L453	Y519	Y604	P696	ASP	GLN	GLN
SER	Y226	Y301	R373	K454	L521	V609	P697	ASP	THR	GLY
GLY	L230	V303	C376	S455	R524	D610	L698	SER	LYS	ASP
VAL	N231	V303	N377	S456	A527	T611	R701	ARG	SER	LYS
ASN	E232	R304	E378	L457	E527	E617	F702	ASP	VAL	VAL
LEU	M233	Y306	P305	K458	P528	S618	D703	GLY	ILE	ILE
ASP	R234	N307	N330	T459	S529	G619	L713	LYS	VAL	VAL
THR	E235	V308	L394	V460	I530	G619	E714	ARG	LEU	GLY
SER	L236	G309	L394	V461	Y531	D625	E714	LYS	GLY	GLY
SER	G237	K312	R388	D462	E532	V628	K715	GLN	GLY	GLY
SER	T238	G313	A392	V463	E534	G629	D717	ASP	VAL	VAL
ALA	N240	N314	A392	H465	E534	C630	D717	ARG	ARG	ARG
PRO	L241	R315	K398	V466	K537	I631	R718	SER	SER	SER
PRO	N242	N318	L398	V467	K538	D632	A721	VAL	VAL	VAL
SER	L243	Q000	L399	L469	Q543	D632	F722	ARG	ARG	ARG
GLY	D244	E401	E401	S470	L544	D635	H723	LEU	LEU	LEU
ALA	A245	K324	E401	S470	F545	K636	I801	ILE	ILE	ASN
SER	R246	T402	T402	D471	F545	K636	I802	ASN	ASN	ASN
GLY	N247	P403	P403	R472	G546	T641	L727	ASN	ASN	ARG
PRO	L248	N327	D404	R473	G547	R642	L728	VAL	VAL	VAL
L177	L249	L328	F405	L474	T548	H646	L729	LEU	LEU	VAL
L178	A250	E329	V406	D475	T548	H646	E730	LYS	LYS	VAL
L179	Q253	G330	P407	V476	R557	E647	E731	ASP	ASP	VAL
L180		L331	D408	D477	F558		K732	GLN	GLN	

## • Molecule 4: Minichromosome Maintenance 5

Chain 5:

45%

36%

18%

MET	T95	I194	V265	S345	MET	S2	F265	S945
S2	I101	N195	P266	F349	S2	F3	P267	
D4	A110	F197	G268	E356	D4	D4	G269	
Q15	ASN	SER	E269	F357	Q15	ASN	E270	
G16	ASN	ILE	P271	N363	G16	ASN	P272	
P19	ASN	T201	R272	L366	P19	ASN	R273	
M20	LYS	V204	M276	A375	M20	LYS	M277	
D21	ASP	V205	C278	P376	D21	ASP	C279	
T25	PRO	P208	L282	I374	T25	PRO	L283	
E26	ASN	R209	L282	A375	E26	ASN	L283	
I28	THR	S210	V286	S377	I28	THR	V287	
K29	MET	C211	I287	I378	K29	MET	I288	
S30	SER	LEU	I287	F379	S30	SER	I288	
F31	THR	SER	T290	K385	F31	THR	T291	
F34	ASP	ILE	R291	K386	F34	ASP	R292	
I35	SER	GLY	T292	A387	I35	SER	T293	
F38	LEU	GLU	V295	I388	F38	LEU	V296	
F44	M130	SER	S299	C390	F44	SER	S300	
I45	L137	ALA	I300	L391	I45	ALA	I301	
Y46	I138	ASN	Y302	L392	Y46	ASN	Y303	
R47	S141	GLY	S303	S396	R47	GLY	S304	
D48	M142	SER	K304	K397	D48	SER	K305	
Q49	A143	ASN	K306	K398	Q49	ASN	K307	
L50	ILE	ILE	G403	D402	L50	ILE	G404	
N53	GLY	GLY	M404	G403	N53	GLY	M405	
T62	P147	LEU	R407	R408	T62	LEU	R409	
R65	L148	GLN	R408	N410	R65	GLN	R409	
E66	R149	SER	D409	V412	E66	SER	D410	
H67	D150	THR	N411	L413	H67	THR	N412	
L68	L151	LYS	N412	L414	L68	LYS	N413	
I69	H155	ASN	D239	L415	I69	ASN	D240	
E73	V156	GLY	P240	S319	E73	GLY	P241	
D74	I165	GLY	Y241	G320	D74	GLY	Y242	
I75	I166	GLY	S247	I330	I75	GLY	S248	
Y76	S170	VAL	T251	L331	Y76	VAL	T252	
K77	L171	ARG	D252	G332	K77	ARG	D253	
L78	L172	ARG	Q253	I333	L78	ARG	Q254	
L79	R175	SER	Q254	V337	L79	SER	Q255	
T86	Y178	VAL	F255	E338	T86	VAL	F256	
I87	L179	LEU	L256	T339	I87	LEU	L257	
P88	S180	ASN	L256	T340	P88	ASN	L257	
L89	I181	ASN	Q259	S440	L89	ASN	Q260	
F90	I181	ARG	E260	S441	F90	ARG	E261	
E91	R184	VAL	T261	I342	E91	VAL	T262	
T92	T193	LYS	E262	K442	T92	LYS	E263	
A93		ASP	E263	G443	A93	ASP	E264	
I94		GLN	L264		I94	GLN	L265	

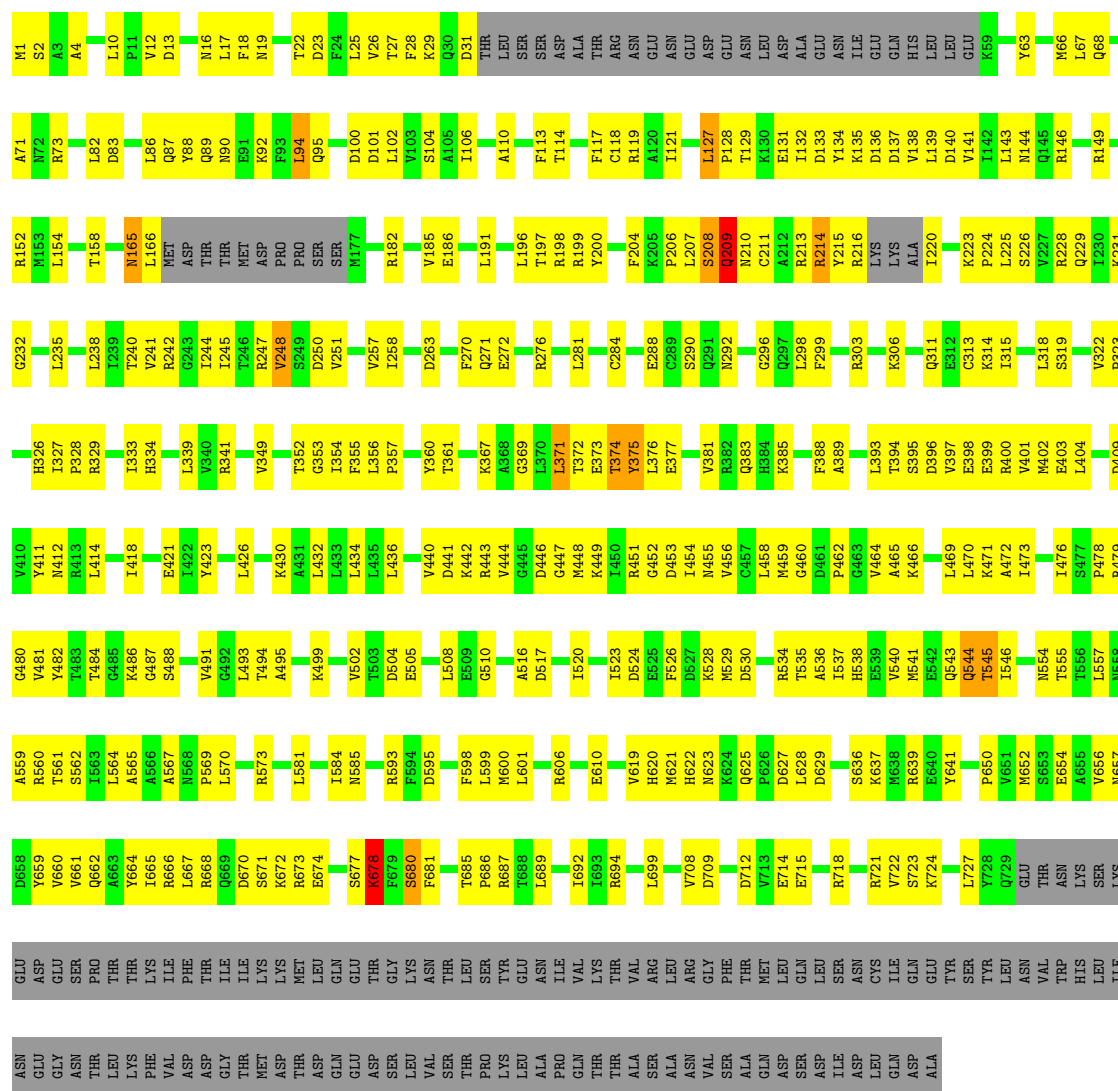




LYS VAL ILE ILE LYS LYS ARG LEU VAL LYS LYS ASP ARG ARG ILE LEU LEU MET GLU ILE ILE HIS GLY THR ARG ARG ASN ASN LEU LEU ARG ASP LEU LEU GLU GLU GLU GLU ASN ASN GLU ASN ASN ASN THR THR TYR VAL VAL VAL ILE ILE HIS HIS PRO PRO CYS ASN ASN VAL VAL VAL VAL LEU LEU LEU GLN LEU LEU PRO PRO GLN GLN ASP ASP SER SER

● Molecule 6: Minichromosome Maintenance 7

Chain 7:  42% 38% • 19%



## 4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	85365	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	CTFFIND	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	22	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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  >2	RMSZ	# Z  >2
1	2	0.41	0/4794	0.64	2/6479 (0.0%)
2	3	0.48	0/4827	0.67	1/6545 (0.0%)
3	4	0.45	0/5154	0.67	4/6967 (0.1%)
4	5	0.46	0/5032	0.62	0/6799
5	6	0.40	0/4812	0.65	1/6497 (0.0%)
6	7	0.47	0/5514	0.65	3/7450 (0.0%)
All	All	0.45	0/30133	0.65	11/40737 (0.0%)

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	2	0	4
2	3	0	2
3	4	0	3
5	6	0	5
6	7	0	5
All	All	0	19

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	654	PRO	CA-N-CD	-8.68	99.35	111.50
5	6	399	GLY	N-CA-C	6.81	130.12	113.10
6	7	127	LEU	CA-CB-CG	6.30	129.79	115.30
6	7	209	GLN	N-CA-C	-6.27	94.06	111.00
3	4	243	LEU	CA-CB-CG	5.94	128.96	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	7	208	SER	N-CA-C	-5.92	95.03	111.00
3	4	376	CYS	C-N-CA	5.62	135.75	121.70
1	2	366	ASN	C-N-CA	5.58	135.64	121.70
1	2	570	GLY	N-CA-C	5.33	126.42	113.10
3	4	727	LEU	CA-CB-CG	5.27	127.41	115.30
3	4	376	CYS	CA-C-N	5.11	128.43	117.20

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	367	CYS	Peptide
1	2	372	PRO	Peptide
1	2	436	GLY	Peptide
1	2	803	PHE	Peptide
2	3	172	THR	Peptide
2	3	428	LEU	Peptide
3	4	352	CYS	Peptide
3	4	373	ARG	Peptide
3	4	408	ASP	Peptide
5	6	133	GLU	Peptide
5	6	338	CYS	Peptide
5	6	344	TRP	Peptide
5	6	398	THR	Peptide
5	6	600	GLY	Peptide
6	7	165	ASN	Peptide
6	7	545	THR	Peptide
6	7	678	LYS	Peptide
6	7	680	SER	Peptide
6	7	94	LEU	Peptide

## 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	2	4714	0	4730	259	0
2	3	4745	0	4793	311	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	4	5081	0	5125	338	0
4	5	4962	0	4994	265	0
5	6	4742	0	4692	317	0
6	7	5432	0	5495	349	0
7	2	27	0	12	1	0
7	3	27	0	12	4	0
7	4	27	0	12	6	0
7	5	27	0	12	7	0
7	6	27	0	12	10	0
7	7	27	0	12	6	0
All	All	29838	0	29901	1676	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 28.

All (1676) 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)
2:3:653:ILE:CD1	4:5:402:ASP:HB3	1.36	1.53
2:3:653:ILE:HD13	4:5:402:ASP:CB	1.55	1.36
2:3:652:THR:C	2:3:654:PRO:HD3	1.52	1.28
2:3:653:ILE:CD1	4:5:402:ASP:CB	2.11	1.26
6:7:214:ARG:HG3	6:7:215:TYR:C	1.64	1.14
5:6:355:ASP:OD2	5:6:383:GLY:N	1.80	1.13
2:3:653:ILE:HD11	4:5:402:ASP:HB3	1.19	1.09
1:2:327:ARG:NH1	4:5:269:GLU:OE2	1.85	1.08
1:2:298:SER:O	1:2:319:ARG:NH1	1.87	1.08
2:3:366:SER:CB	2:3:651:VAL:HG13	1.83	1.07
2:3:366:SER:HB3	2:3:651:VAL:HG13	1.09	1.06
2:3:43:ARG:HH12	2:3:137:ASP:HB2	1.17	1.05
2:3:654:PRO:HD2	2:3:655:PHE:H	1.17	1.05
6:7:662:GLN:HB3	6:7:666:ARG:HH12	1.18	1.05
2:3:652:THR:C	2:3:654:PRO:CD	2.25	1.04
2:3:652:THR:O	2:3:654:PRO:HD2	1.57	1.04
2:3:652:THR:O	2:3:654:PRO:CD	2.05	1.04
6:7:453:ASP:OD2	6:7:562:SER:OG	1.75	1.04
4:5:442:LYS:NZ	4:5:484:LYS:O	1.92	1.02
6:7:149:ARG:NH1	6:7:152:ARG:HH11	1.59	1.00
2:3:409:GLY:O	2:3:415:LYS:NZ	1.95	1.00
6:7:460:GLY:O	6:7:466:LYS:NZ	1.94	0.99
1:2:614:ASP:OD1	1:2:617:ARG:NH1	1.96	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:506:LEU:HB3	3:4:510:ARG:HH12	1.28	0.99
2:3:234:GLU:OE2	2:3:240:LYS:NZ	1.95	0.98
5:6:566:ARG:NH1	5:6:656:MET:O	1.97	0.98
3:4:315:ARG:HH12	6:7:251:VAL:N	1.60	0.98
2:3:569:HIS:O	4:5:398:LYS:NZ	1.97	0.97
2:3:653:ILE:CD1	4:5:402:ASP:CA	2.41	0.97
6:7:118:CYS:SG	6:7:198:ARG:NH1	2.37	0.97
1:2:656:ARG:HH11	5:6:794:ARG:HA	1.28	0.96
6:7:715:GLU:OE2	6:7:718:ARG:NH1	1.96	0.96
4:5:349:PHE:HB3	4:5:601:ARG:HH21	1.30	0.96
2:3:653:ILE:HD13	4:5:402:ASP:HB3	1.09	0.95
1:2:522:GLY:O	1:2:822:LYS:NZ	1.99	0.95
2:3:420:ARG:NH1	4:5:495:GLU:OE2	1.99	0.95
2:3:391:LYS:NZ	6:7:623:ASN:OD1	2.00	0.94
2:3:519:VAL:HG22	2:3:534:ALA:HB2	1.47	0.94
6:7:214:ARG:NH2	6:7:214:ARG:HB2	1.82	0.94
3:4:315:ARG:HH12	6:7:251:VAL:H	0.99	0.94
2:3:195:LYS:NZ	6:7:369:GLY:O	2.00	0.94
4:5:426:LEU:HD21	4:5:520:LEU:HD22	1.50	0.93
2:3:366:SER:HB3	2:3:651:VAL:CG1	1.98	0.93
3:4:647:GLU:OE2	3:4:655:SER:N	2.02	0.93
2:3:43:ARG:NH1	2:3:137:ASP:HB2	1.85	0.91
5:6:575:GLY:O	5:6:581:LYS:NZ	2.04	0.91
2:3:389:VAL:HG12	2:3:390:GLU:H	1.32	0.90
3:4:428:ARG:HH12	3:4:482:GLU:HG3	1.36	0.90
6:7:94:LEU:HB2	6:7:95:GLN:HB2	1.52	0.90
1:2:433:ASN:HB2	1:2:434:TYR:HB2	1.52	0.90
5:6:183:LYS:HG2	5:6:186:ARG:HH11	1.34	0.90
5:6:355:ASP:HB3	5:6:356:TRP:HA	1.54	0.90
6:7:208:SER:HB3	6:7:209:GLN:CB	2.02	0.89
2:3:216:ASP:OD1	2:3:219:THR:N	2.06	0.89
4:5:606:CYS:O	4:5:665:LYS:NZ	2.05	0.89
2:3:519:VAL:HB	2:3:527:ARG:HH12	1.38	0.88
5:6:691:ARG:HH11	5:6:716:LEU:HD22	1.38	0.88
4:5:375:ALA:HB1	4:5:378:ILE:HB	1.56	0.87
5:6:133:GLU:HB3	5:6:134:LYS:HA	1.55	0.86
4:5:551:ASP:OD2	4:5:658:ARG:NH2	2.09	0.86
3:4:202:LYS:HA	3:4:224:LEU:HA	1.57	0.86
3:4:557:ARG:HH11	3:4:668:ARG:NH2	1.74	0.86
6:7:315:ILE:HD13	6:7:333:ILE:HD12	1.57	0.86
3:4:211:GLU:OE2	3:4:212:ARG:NH1	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:255:ARG:NH2	2:3:275:ASP:OD2	2.07	0.85
6:7:288:GLU:O	6:7:292:ASN:ND2	2.09	0.85
2:3:212:ARG:HH11	2:3:229:ALA:HB1	1.39	0.85
5:6:778:LYS:HG2	5:6:782:LYS:HZ2	1.39	0.85
5:6:586:LYS:NZ	5:6:597:TYR:OH	2.09	0.85
2:3:24:ARG:NH1	2:3:120:TYR:HB3	1.91	0.85
1:2:425:GLU:HB3	1:2:457:LYS:HB2	1.59	0.84
5:6:778:LYS:O	5:6:782:LYS:NZ	2.09	0.84
3:4:666:ASN:HD22	3:4:668:ARG:HH22	1.26	0.84
1:2:656:ARG:NH1	5:6:794:ARG:HA	1.91	0.84
1:2:327:ARG:NH1	1:2:420:PRO:HD3	1.92	0.84
5:6:296:ARG:HE	5:6:613:VAL:HG21	1.43	0.84
3:4:731:ASP:O	6:7:442:LYS:NZ	2.10	0.84
1:2:543:GLY:HA3	1:2:549:LYS:HD3	1.58	0.84
5:6:558:SER:HB3	5:6:559:THR:HA	1.57	0.84
2:3:653:ILE:N	2:3:654:PRO:HD3	1.91	0.84
6:7:73:ARG:NH1	6:7:136:ASP:OD1	2.10	0.83
5:6:737:LYS:O	5:6:738:ARG:NH1	2.11	0.83
2:3:654:PRO:HD2	2:3:655:PHE:N	1.91	0.83
1:2:299:ASP:HA	1:2:319:ARG:NH1	1.93	0.83
2:3:368:ALA:HB2	2:3:378:LYS:HE2	1.60	0.83
6:7:16:ASN:ND2	6:7:100:ASP:OD2	2.12	0.83
3:4:506:LEU:HB3	3:4:510:ARG:NH1	1.93	0.83
5:6:621:TYR:HB3	5:6:668:ILE:HD13	1.61	0.83
1:2:297:ILE:HG22	1:2:298:SER:H	1.43	0.83
6:7:73:ARG:O	6:7:199:ARG:NH1	2.11	0.83
4:5:197:PHE:HZ	4:5:251:ILE:HD11	1.45	0.82
5:6:296:ARG:HH12	5:6:360:ARG:NH1	1.76	0.82
2:3:653:ILE:HD13	4:5:402:ASP:CA	2.05	0.82
1:2:690:GLU:OE2	1:2:694:ARG:NE	2.13	0.82
3:4:432:ARG:NH1	3:4:586:PRO:O	2.12	0.82
3:4:489:LYS:NZ	3:4:497:GLU:HB2	1.94	0.81
2:3:559:ARG:HH21	4:5:627:VAL:HG21	1.45	0.81
6:7:453:ASP:OD1	6:7:454:ILE:N	2.13	0.81
3:4:602:THR:HA	3:4:619:GLY:HA3	1.63	0.81
3:4:651:GLN:NE2	5:6:597:TYR:OH	2.13	0.81
1:2:243:GLU:OE2	1:2:298:SER:OG	1.98	0.80
2:3:291:ARG:HH11	4:5:511:THR:HG22	1.46	0.80
3:4:362:ARG:NH1	6:7:263:ASP:OD2	2.14	0.80
3:4:334:ARG:NH2	3:4:617:GLU:OE2	2.14	0.80
3:4:326:ILE:HD12	3:4:439:PHE:HB2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:828:TYR:OH	5:6:832:ARG:NH2	2.13	0.80
5:6:796:THR:HG22	5:6:798:ARG:H	1.46	0.80
6:7:662:GLN:HB3	6:7:666:ARG:NH1	1.97	0.80
3:4:188:GLN:O	3:4:190:CYS:N	2.14	0.80
4:5:264:LEU:HB2	4:5:265:VAL:HG22	1.64	0.80
6:7:208:SER:HB3	6:7:209:GLN:CG	2.11	0.80
3:4:234:ARG:NH1	3:4:284:ILE:HG13	1.95	0.80
3:4:401:GLU:OE2	3:4:413:HIS:HB3	1.80	0.80
1:2:401:ARG:HG3	5:6:390:LYS:NZ	1.95	0.80
1:2:309:LEU:O	1:2:310:ARG:NH1	2.13	0.79
2:3:437:SER:HB3	2:3:438:SER:HA	1.63	0.79
6:7:443:ARG:HH12	6:7:449:LYS:NZ	1.81	0.79
2:3:654:PRO:CD	2:3:655:PHE:H	1.95	0.79
4:5:608:LEU:HD11	4:5:609:LYS:NZ	1.97	0.79
3:4:315:ARG:NH1	6:7:251:VAL:H	1.79	0.79
1:2:274:VAL:HG13	1:2:277:GLU:OE2	1.82	0.78
6:7:361:THR:HG21	6:7:367:LYS:HD2	1.64	0.78
3:4:604:TYR:HE2	6:7:554:ASN:HD21	1.29	0.78
5:6:790:ARG:NH1	5:6:839:ASP:OD2	2.16	0.78
5:6:597:TYR:OH	5:6:639:ASP:OD2	2.01	0.78
6:7:504:ASP:HB3	6:7:505:GLU:HB3	1.66	0.78
5:6:689:TYR:HA	5:6:690:ASN:HB2	1.64	0.78
2:3:366:SER:CB	2:3:651:VAL:CG1	2.59	0.77
3:4:713:ASP:HB2	3:4:716:ASN:HB2	1.65	0.77
6:7:87:GLN:HE22	6:7:214:ARG:NH1	1.81	0.77
3:4:406:VAL:HG23	6:7:560:ARG:HH12	1.49	0.77
2:3:559:ARG:HE	4:5:627:VAL:HG11	1.50	0.77
1:2:339:PHE:HB2	1:2:348:LEU:HD23	1.65	0.77
2:3:336:VAL:HG12	2:3:337:ALA:HA	1.66	0.77
5:6:183:LYS:CG	5:6:186:ARG:HH11	1.98	0.77
5:6:691:ARG:NH1	5:6:716:LEU:HD22	2.00	0.77
1:2:502:ALA:HB3	1:2:512:LYS:HE2	1.67	0.77
2:3:653:ILE:CD1	4:5:402:ASP:HA	2.15	0.76
1:2:327:ARG:HH12	1:2:420:PRO:HD3	1.49	0.76
2:3:230:ILE:HG22	2:3:231:TYR:H	1.51	0.76
4:5:170:SER:O	4:5:254:GLN:NE2	2.17	0.76
5:6:792:SER:HA	5:6:793:TYR:HB2	1.67	0.76
6:7:214:ARG:N	6:7:215:TYR:HA	2.00	0.76
5:6:580:SER:N	7:6:2001:ADP:O1A	2.17	0.75
5:6:691:ARG:HE	5:6:716:LEU:HD13	1.48	0.75
6:7:374:THR:OG1	6:7:375:TYR:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:677:SER:OG	6:7:678:LYS:N	2.19	0.75
2:3:653:ILE:HD11	4:5:402:ASP:CB	1.95	0.75
6:7:530:ASP:O	6:7:534:ARG:NH1	2.18	0.75
6:7:23:ASP:O	6:7:27:THR:OG1	2.02	0.75
2:3:212:ARG:NH1	2:3:229:ALA:HB1	2.02	0.75
4:5:407:ARG:NH2	4:5:658:ARG:HH12	1.85	0.75
6:7:86:LEU:HD12	6:7:216:ARG:HG2	1.69	0.75
3:4:352:CYS:N	3:4:373:ARG:O	2.19	0.75
2:3:414:ALA:N	7:3:2001:ADP:O1A	2.20	0.74
3:4:650:GLU:CD	3:4:796:ARG:HH12	1.90	0.74
6:7:455:ASN:ND2	6:7:541:MET:SD	2.60	0.74
1:2:523:VAL:HG12	1:2:525:LYS:HB3	1.68	0.74
6:7:87:GLN:HE22	6:7:214:ARG:HH12	1.33	0.74
2:3:291:ARG:NH1	4:5:511:THR:HG22	2.02	0.74
4:5:538:ASP:H	4:5:544:THR:HG22	1.52	0.74
1:2:507:GLY:HA3	1:2:512:LYS:HE3	1.70	0.74
2:3:684:THR:HG21	6:7:610:GLU:OE2	1.87	0.74
5:6:426:ILE:HG22	5:6:427:SER:H	1.51	0.74
6:7:443:ARG:NH1	6:7:449:LYS:NZ	2.35	0.74
4:5:204:THR:HG22	4:5:205:VAL:HG23	1.69	0.74
5:6:776:LYS:O	5:6:779:GLU:HG2	1.88	0.74
6:7:214:ARG:HG3	6:7:215:TYR:O	1.86	0.74
3:4:594:LYS:HG3	6:7:535:THR:HG21	1.68	0.74
2:3:553:ILE:HB	4:5:630:ARG:HD2	1.68	0.74
5:6:296:ARG:NH1	5:6:360:ARG:NH1	2.36	0.74
3:4:575:SER:OG	7:4:2001:ADP:O2A	2.06	0.74
3:4:333:LEU:HD12	3:4:398:LYS:HZ2	1.51	0.74
1:2:253:LYS:HE2	1:2:256:LEU:HD11	1.68	0.74
3:4:408:ASP:CG	3:4:409:GLY:HA2	2.08	0.74
5:6:533:ILE:HD12	5:6:544:LYS:HB3	1.70	0.73
3:4:561:ASP:O	3:4:803:ARG:NH2	2.22	0.73
2:3:519:VAL:HB	2:3:527:ARG:NH1	2.03	0.73
3:4:764:GLU:HA	3:4:767:LYS:NZ	2.02	0.73
3:4:348:LYS:HB3	3:4:353:ASP:OD2	1.89	0.73
4:5:608:LEU:HD11	4:5:609:LYS:HZ2	1.53	0.73
5:6:819:ILE:HG22	5:6:820:THR:H	1.54	0.73
2:3:362:ILE:CG2	2:3:651:VAL:HG21	2.17	0.73
3:4:234:ARG:HE	3:4:291:TYR:HE2	1.36	0.73
5:6:538:PHE:H	7:6:2001:ADP:HN62	1.35	0.73
5:6:566:ARG:HH21	5:6:659:GLN:HB2	1.52	0.73
2:3:314:LEU:O	4:5:175:ARG:NH2	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:712:VAL:HG22	6:7:672:LYS:NZ	2.03	0.72
4:5:379:PHE:H	7:5:2001:ADP:HN62	1.34	0.72
4:5:455:ARG:NH1	4:5:460:ARG:HB3	2.02	0.72
6:7:208:SER:HB3	6:7:209:GLN:HB2	1.69	0.72
5:6:582:SER:HA	5:6:585:LEU:HD12	1.69	0.72
6:7:154:LEU:HD21	6:7:191:LEU:HD11	1.71	0.72
2:3:159:GLY:HA2	2:3:160:SER:HB2	1.71	0.72
3:4:484:GLU:O	3:4:488:ASN:N	2.21	0.72
3:4:512:VAL:HG13	3:4:515:ARG:NH1	2.03	0.72
6:7:214:ARG:HH21	6:7:214:ARG:HB2	1.51	0.72
1:2:300:PHE:O	1:2:302:THR:OG1	2.06	0.72
6:7:198:ARG:NH2	6:7:200:TYR:OH	2.20	0.72
6:7:73:ARG:HD2	6:7:140:ASP:OD2	1.90	0.72
6:7:214:ARG:HG3	6:7:215:TYR:CA	2.18	0.72
7:4:2001:ADP:O3A	6:7:687:ARG:NH2	2.22	0.72
3:4:458:LYS:NZ	5:6:413:PRO:HB3	2.04	0.72
4:5:588:GLU:O	4:5:593:GLU:N	2.23	0.72
2:3:163:ALA:H	2:3:164:HIS:HB2	1.55	0.72
3:4:370:ARG:HB2	3:4:371:CYS:HB2	1.70	0.72
3:4:592:SER:HA	3:4:632:ASP:HB2	1.71	0.72
6:7:73:ARG:NH1	6:7:140:ASP:OD2	2.23	0.72
2:3:722:ASN:OD1	2:3:723:LYS:N	2.21	0.72
2:3:49:ASN:OD1	2:3:91:ILE:N	2.22	0.72
3:4:353:ASP:OD1	3:4:354:HIS:N	2.23	0.71
3:4:527:ALA:HB3	3:4:537:LYS:NZ	2.05	0.71
5:6:183:LYS:NZ	5:6:186:ARG:NH1	2.38	0.71
2:3:449:ASP:OD1	2:3:453:GLY:HA2	1.90	0.71
6:7:165:ASN:HB3	6:7:166:LEU:HA	1.71	0.71
2:3:113:GLY:HA3	2:3:121:PHE:CE2	2.26	0.71
6:7:228:ARG:NH2	6:7:327:ILE:O	2.23	0.71
6:7:385:LYS:HA	6:7:639:ARG:NH1	2.06	0.71
2:3:347:ILE:O	2:3:351:ASN:ND2	2.24	0.71
3:4:610:ASP:OD1	3:4:611:THR:N	2.23	0.71
6:7:443:ARG:HH12	6:7:449:LYS:HZ1	1.37	0.71
3:4:557:ARG:HH11	3:4:668:ARG:HH21	1.39	0.70
3:4:701:ARG:NH2	7:6:2001:ADP:O3B	2.24	0.70
3:4:767:LYS:HG2	5:6:732:VAL:HG11	1.72	0.70
1:2:242:LEU:HB3	1:2:295:VAL:HG12	1.74	0.70
2:3:440:VAL:HG21	2:3:482:ASP:OD2	1.91	0.70
2:3:362:ILE:CG2	2:3:651:VAL:CG2	2.69	0.70
4:5:407:ARG:CZ	4:5:658:ARG:HH12	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:149:ARG:NH1	6:7:152:ARG:NH1	2.37	0.70
6:7:146:ARG:NH1	6:7:196:LEU:HD21	2.06	0.70
2:3:689:ASP:O	2:3:692:THR:OG1	2.10	0.70
1:2:325:THR:HG22	1:2:326:ARG:H	1.56	0.69
2:3:400:ARG:NH2	2:3:544:ASP:OD1	2.24	0.69
3:4:762:ILE:HG12	5:6:736:MET:HE3	1.73	0.69
1:2:766:TYR:OH	1:2:823:MET:O	2.10	0.69
1:2:843:ASP:OD1	1:2:844:SER:N	2.25	0.69
2:3:212:ARG:NH1	2:3:229:ALA:O	2.24	0.69
3:4:259:HIS:ND1	6:7:135:LYS:HE3	2.06	0.69
2:3:420:ARG:NH2	4:5:501:THR:OG1	2.21	0.69
6:7:482:TYR:OH	6:7:524:ASP:OD2	2.03	0.69
1:2:441:LYS:HA	1:2:442:ASN:HB2	1.74	0.69
3:4:512:VAL:HG13	3:4:515:ARG:HH12	1.57	0.69
5:6:288:LEU:H	5:6:399:GLY:HA3	1.57	0.69
1:2:299:ASP:HA	1:2:319:ARG:HH12	1.55	0.69
1:2:839:LYS:NZ	1:2:864:TYR:HA	2.07	0.69
4:5:78:LYS:HG3	4:5:86:ILE:HD11	1.74	0.69
5:6:301:ARG:NH2	5:6:618:GLY:O	2.25	0.69
1:2:241:SER:OG	1:2:413:ASP:OD2	2.10	0.69
3:4:428:ARG:NH1	3:4:482:GLU:HA	2.06	0.69
3:4:483:GLN:HG3	3:4:484:GLU:H	1.56	0.69
2:3:654:PRO:O	2:3:658:LYS:NZ	2.26	0.69
5:6:123:SER:HB2	5:6:135:VAL:H	1.57	0.69
2:3:113:GLY:HA3	2:3:121:PHE:HE2	1.57	0.69
2:3:451:GLU:HG3	2:3:452:THR:HG23	1.75	0.69
3:4:727:LEU:N	3:4:728:TYR:HB3	2.09	0.68
2:3:520:PHE:HE1	4:5:542:PHE:HB3	1.58	0.68
3:4:354:HIS:HD2	3:4:372:GLU:HG3	1.57	0.68
3:4:774:TYR:OH	3:4:778:ARG:NH2	2.26	0.68
4:5:375:ALA:H	4:5:385:LYS:HE3	1.58	0.68
1:2:780:GLN:NE2	4:5:577:THR:O	2.27	0.68
5:6:575:GLY:N	5:6:581:LYS:HZ3	1.90	0.68
6:7:484:THR:HG23	6:7:487:GLY:HA2	1.76	0.68
2:3:260:GLU:OE2	2:3:271:PRO:HA	1.94	0.68
2:3:53:ALA:O	2:3:57:ASN:ND2	2.27	0.68
3:4:489:LYS:HZ1	3:4:497:GLU:HB2	1.59	0.68
5:6:609:THR:HG22	5:6:610:ALA:H	1.59	0.68
1:2:583:ASP:HB3	1:2:587:LYS:HE3	1.76	0.68
2:3:570:ARG:HB3	4:5:613:ARG:HH21	1.58	0.68
3:4:714:GLU:H	3:4:715:LYS:HB3	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:830:ARG:HD3	3:4:833:ILE:HD12	1.76	0.67
4:5:375:ALA:N	4:5:385:LYS:HE3	2.09	0.67
4:5:461:GLU:HG2	4:5:462:PHE:H	1.59	0.67
4:5:570:ASN:O	4:5:574:ASN:ND2	2.27	0.67
5:6:625:ALA:HB3	5:6:626:GLY:HA2	1.74	0.67
2:3:716:ARG:HH22	2:3:724:VAL:HB	1.57	0.67
5:6:540:HIS:O	5:6:542:ALA:N	2.27	0.67
5:6:600:GLY:HA2	5:6:602:ALA:N	2.08	0.67
6:7:247:ARG:HG2	6:7:314:LYS:NZ	2.08	0.67
1:2:549:LYS:HE3	7:2:2001:ADP:O2B	1.94	0.67
3:4:563:ASN:ND2	3:4:649:MET:SD	2.68	0.67
5:6:759:ARG:HA	5:6:812:ARG:HH21	1.59	0.67
6:7:388:PHE:HB2	6:7:389:ALA:HA	1.75	0.67
4:5:178:TYR:HD1	4:5:193:THR:HG22	1.59	0.67
6:7:228:ARG:HE	6:7:329:ARG:HG3	1.59	0.67
2:3:163:ALA:HB3	2:3:164:HIS:HD1	1.59	0.67
2:3:48:TYR:O	2:3:52:ASN:ND2	2.24	0.67
4:5:166:ILE:HD12	4:5:286:VAL:HG11	1.77	0.67
5:6:183:LYS:HZ2	5:6:186:ARG:NH1	1.93	0.67
2:3:101:ASP:HA	2:3:104:ARG:HH21	1.59	0.67
6:7:104:SER:OG	6:7:216:ARG:NH1	2.27	0.67
1:2:601:LYS:NZ	1:2:643:ARG:HD2	2.11	0.66
2:3:276:VAL:HG22	2:3:321:ILE:HB	1.77	0.66
6:7:652:MET:HG2	6:7:708:VAL:HG11	1.77	0.66
1:2:338:LYS:HE2	1:2:379:LYS:HB2	1.77	0.66
2:3:651:VAL:O	2:3:651:VAL:HG12	1.94	0.66
5:6:767:LYS:HE3	5:6:769:ALA:HB3	1.77	0.66
6:7:444:VAL:HG22	6:7:448:MET:H	1.60	0.66
5:6:781:ARG:HG2	5:6:795:ILE:HB	1.78	0.66
6:7:593:ARG:HG2	6:7:687:ARG:NH1	2.10	0.66
1:2:394:PRO:O	5:6:673:ASN:ND2	2.28	0.66
3:4:717:ASP:OD2	6:7:668:ARG:HG2	1.96	0.66
5:6:179:PRO:HA	5:6:182:GLN:NE2	2.10	0.66
1:2:309:LEU:H	1:2:310:ARG:NH1	1.94	0.66
1:2:678:ASP:OD1	1:2:679:ILE:N	2.29	0.66
5:6:399:GLY:HA2	5:6:454:PHE:CZ	2.31	0.66
2:3:24:ARG:HH12	2:3:120:TYR:HB3	1.58	0.65
3:4:188:GLN:C	3:4:190:CYS:H	2.00	0.65
2:3:163:ALA:N	2:3:164:HIS:HB2	2.10	0.65
2:3:476:ASP:O	2:3:483:ARG:NH1	2.29	0.65
2:3:696:PRO:HB3	6:7:573:ARG:HH12	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:393:LEU:HA	6:7:394:THR:HB	1.77	0.65
6:7:670:ASP:OD1	6:7:671:SER:N	2.30	0.65
3:4:226:TYR:OH	3:4:247:ASN:ND2	2.22	0.65
2:3:95:ARG:NE	2:3:281:ASP:OD2	2.27	0.65
6:7:247:ARG:HG2	6:7:314:LYS:HZ1	1.60	0.65
2:3:189:THR:HG22	2:3:190:SER:H	1.61	0.65
2:3:33:ASP:CB	2:3:39:ARG:HH11	2.09	0.65
3:4:714:GLU:N	3:4:715:LYS:HB3	2.11	0.65
6:7:543:GLN:HG3	6:7:544:GLN:H	1.60	0.65
2:3:476:ASP:HA	2:3:483:ARG:HH12	1.61	0.65
3:4:532:GLU:HG2	3:4:533:LEU:H	1.59	0.65
4:5:301:TYR:CE1	4:5:303:SER:HB3	2.31	0.65
2:3:524:ASP:OD1	2:3:532:ASN:ND2	2.30	0.65
3:4:349:CYS:H	3:4:353:ASP:CG	2.01	0.65
5:6:541:GLU:O	5:6:545:LYS:NZ	2.28	0.65
2:3:553:ILE:HD11	4:5:634:LEU:HD13	1.80	0.64
2:3:119:ALA:HA	2:3:221:LEU:HD22	1.79	0.64
2:3:525:VAL:HG11	2:3:552:ASP:OD2	1.97	0.64
3:4:360:ILE:HG13	3:4:365:ILE:HG12	1.79	0.64
4:5:149:ARG:NH1	4:5:272:ARG:HE	1.95	0.64
6:7:67:LEU:HD11	6:7:121:ILE:HG23	1.79	0.64
3:4:370:ARG:HH12	5:6:426:ILE:CG1	2.10	0.64
2:3:410:ASP:O	2:3:413:THR:OG1	2.11	0.64
3:4:703:ASP:OD1	3:4:800:SER:OG	2.08	0.64
3:4:650:GLU:OE1	3:4:796:ARG:NH1	2.31	0.64
5:6:596:VAL:HG23	5:6:631:ALA:HB2	1.79	0.64
5:6:776:LYS:HD3	5:6:828:TYR:HB2	1.79	0.64
1:2:601:LYS:NZ	1:2:643:ARG:NH1	2.45	0.64
4:5:209:ARG:HA	4:5:239:ASP:HB3	1.78	0.64
1:2:495:ASP:CG	1:2:509:ARG:HH12	2.00	0.64
1:2:811:GLU:OE2	1:2:815:ARG:NH1	2.31	0.64
2:3:542:ARG:NH1	2:3:700:ARG:NH1	2.45	0.64
3:4:408:ASP:OD2	3:4:409:GLY:HA2	1.97	0.64
6:7:220:ILE:HA	6:7:223:LYS:NZ	2.13	0.64
6:7:662:GLN:CB	6:7:666:ARG:HH12	2.02	0.64
1:2:289:ILE:HG22	1:2:290:HIS:CD2	2.33	0.64
2:3:268:GLY:O	2:3:269:GLN:HG3	1.97	0.64
3:4:573:SER:N	7:4:2001:ADP:O1A	2.25	0.64
5:6:300:VAL:HG22	5:6:357:GLN:HB3	1.78	0.64
5:6:531:ARG:HD2	5:6:745:PRO:HG3	1.80	0.64
6:7:149:ARG:HH11	6:7:152:ARG:HE	1.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:423:TYR:O	7:7:2001:ADP:N6	2.31	0.64
1:2:286:TYR:HE2	1:2:293:ILE:HD11	1.61	0.64
1:2:505:ILE:HG22	1:2:507:GLY:H	1.62	0.64
3:4:471:ASP:OD1	3:4:472:LYS:N	2.31	0.64
4:5:172:LEU:HD13	4:5:252:ASP:OD2	1.98	0.64
1:2:401:ARG:HG3	5:6:390:LYS:HZ2	1.61	0.63
1:2:792:ASP:O	1:2:859:ARG:NH1	2.31	0.63
1:2:401:ARG:HG3	5:6:390:LYS:HZ3	1.62	0.63
1:2:524:PRO:HB2	1:2:525:LYS:HA	1.79	0.63
2:3:100:LEU:HB3	2:3:111:TRP:HZ3	1.62	0.63
2:3:400:ARG:HG3	2:3:493:GLN:OE1	1.98	0.63
4:5:392:LEU:O	4:5:607:ARG:NH2	2.30	0.63
5:6:183:LYS:HG2	5:6:186:ARG:NH1	2.11	0.63
5:6:775:GLU:O	5:6:779:GLU:N	2.31	0.63
4:5:457:PRO:O	4:5:460:ARG:NH2	2.31	0.63
2:3:390:GLU:HG2	2:3:509:ARG:HH12	1.64	0.63
3:4:186:SER:HB2	3:4:189:GLU:OE2	1.98	0.63
1:2:505:ILE:HD13	1:2:552:ILE:HG13	1.79	0.63
2:3:654:PRO:CD	2:3:655:PHE:N	2.58	0.63
4:5:564:ARG:O	4:5:567:SER:OG	2.13	0.63
6:7:226:SER:HB3	6:7:229:GLN:HG2	1.80	0.63
1:2:526:ASN:HA	1:2:532:SER:HA	1.81	0.63
2:3:199:SER:OG	2:3:201:HIS:NE2	2.32	0.63
3:4:234:ARG:HH12	3:4:284:ILE:HG13	1.62	0.63
6:7:459:MET:C	6:7:466:LYS:HZ3	2.01	0.63
2:3:701:THR:O	2:3:704:THR:OG1	2.14	0.63
6:7:538:HIS:CD2	6:7:593:ARG:HE	2.17	0.63
1:2:540:LEU:HB2	1:2:677:PHE:CD2	2.33	0.62
2:3:445:ALA:HB3	2:3:499:LYS:HD2	1.81	0.62
4:5:178:TYR:CD1	4:5:193:THR:HG22	2.33	0.62
6:7:668:ARG:HH12	6:7:685:THR:HA	1.64	0.62
1:2:383:ARG:HE	1:2:411:LEU:HD23	1.64	0.62
5:6:355:ASP:HB3	5:6:356:TRP:CA	2.24	0.62
1:2:309:LEU:H	1:2:310:ARG:HH12	1.47	0.62
3:4:428:ARG:NH1	3:4:482:GLU:HG3	2.10	0.62
1:2:796:GLU:OE1	1:2:859:ARG:NE	2.30	0.62
3:4:444:ILE:HG21	5:6:411:GLY:HA2	1.81	0.62
3:4:658:LYS:HB3	5:6:604:SER:H	1.63	0.62
3:4:365:ILE:HD12	5:6:448:LEU:HD21	1.82	0.62
6:7:208:SER:OG	6:7:209:GLN:HA	2.00	0.62
6:7:211:CYS:O	6:7:214:ARG:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:235:GLY:HA2	1:2:283:TYR:HE2	1.65	0.62
2:3:734:ARG:O	2:3:738:LEU:N	2.24	0.62
4:5:165:ILE:HD11	4:5:291:ARG:NH1	2.15	0.62
3:4:651:GLN:HE21	5:6:586:LYS:NZ	1.97	0.62
1:2:319:ARG:HE	1:2:427:THR:HG22	1.64	0.62
1:2:338:LYS:NZ	1:2:376:ASN:HD21	1.97	0.62
2:3:269:GLN:HE21	4:5:287:ILE:HG23	1.64	0.62
4:5:388:ILE:HD11	4:5:425:LEU:HD21	1.82	0.62
6:7:491:VAL:HA	6:7:494:THR:HG22	1.80	0.62
2:3:467:ARG:NH1	2:3:509:ARG:CZ	2.63	0.61
6:7:357:PRO:HA	6:7:374:THR:HA	1.81	0.61
6:7:543:GLN:O	6:7:545:THR:N	2.33	0.61
3:4:543:GLN:HA	3:4:562:ILE:HD11	1.82	0.61
4:5:147:PRO:HG2	4:5:150:ASP:HB2	1.82	0.61
4:5:357:PHE:CE1	4:5:598:LYS:HE2	2.36	0.61
3:4:458:LYS:HZ3	5:6:413:PRO:HB3	1.63	0.61
1:2:778:LEU:HG	4:5:577:THR:HG22	1.82	0.61
5:6:550:GLN:HA	5:6:569:ILE:HG21	1.81	0.61
5:6:412:LEU:HB3	5:6:416:LYS:NZ	2.15	0.61
5:6:522:ASP:HB2	5:6:525:ILE:HG23	1.82	0.61
6:7:680:SER:HB2	6:7:681:PHE:HA	1.81	0.61
6:7:149:ARG:NH1	6:7:152:ARG:HE	1.97	0.61
2:3:30:GLU:O	2:3:34:THR:N	2.27	0.61
6:7:465:ALA:HA	7:7:2001:ADP:H5'1	1.83	0.61
6:7:718:ARG:HA	6:7:721:ARG:NH1	2.14	0.61
2:3:27:ARG:NH2	2:3:107:ASP:OD1	2.33	0.61
5:6:611:ALA:H	5:6:624:GLU:HG2	1.66	0.61
1:2:212:LYS:HG3	1:2:274:VAL:CG1	2.31	0.61
3:4:196:ASN:OD1	3:4:197:PHE:N	2.34	0.61
4:5:626:PHE:CG	4:5:653:LEU:HD12	2.36	0.61
2:3:119:ALA:HB1	2:3:222:THR:HG22	1.82	0.61
3:4:688:VAL:O	3:4:691:ASN:N	2.33	0.61
3:4:712:VAL:HG22	6:7:672:LYS:HZ3	1.65	0.61
4:5:441:GLY:HA3	4:5:443:GLY:N	2.16	0.60
1:2:212:LYS:HE3	1:2:274:VAL:HB	1.83	0.60
3:4:475:ASP:OD1	3:4:476:VAL:N	2.33	0.60
5:6:382:ARG:HH11	5:6:455:LEU:HD21	1.64	0.60
6:7:526:PHE:HB3	6:7:567:ALA:HB2	1.83	0.60
2:3:444:ALA:HA	2:3:499:LYS:HZ1	1.66	0.60
3:4:515:ARG:HG2	3:4:517:ASP:OD1	2.01	0.60
3:4:758:ILE:HG22	3:4:760:PRO:HD3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:370:SER:OG	4:5:404:MET:SD	2.58	0.60
1:2:343:LYS:HZ3	1:2:371:GLY:CA	2.15	0.60
1:2:382:TYR:HD2	4:5:156:VAL:HG21	1.66	0.60
1:2:653:ASN:O	1:2:658:ASN:ND2	2.34	0.60
3:4:548:THR:N	3:4:806:GLU:OE2	2.33	0.60
5:6:296:ARG:HH12	5:6:360:ARG:HH11	1.47	0.60
1:2:687:VAL:HG13	1:2:692:ASP:OD2	2.02	0.60
2:3:428:LEU:HB3	2:3:429:ALA:CA	2.31	0.60
5:6:750:GLN:HA	5:6:753:ARG:NH1	2.16	0.60
6:7:248:VAL:HG23	6:7:313:CYS:HB3	1.83	0.60
5:6:183:LYS:NZ	5:6:186:ARG:HH12	2.00	0.60
6:7:451:ARG:O	6:7:694:ARG:NH2	2.32	0.60
1:2:335:LYS:HB3	1:2:381:VAL:O	2.02	0.60
1:2:684:ARG:HB3	1:2:685:ASP:HA	1.83	0.60
3:4:292:ASP:HA	3:4:293:LEU:HD12	1.83	0.60
3:4:493:ASN:O	3:4:494:GLU:HG2	2.00	0.60
4:5:196:ASN:OD1	4:5:197:PHE:N	2.34	0.60
5:6:610:ALA:HB3	5:6:663:ILE:HD13	1.84	0.60
6:7:224:PRO:HB2	6:7:242:ARG:HE	1.67	0.60
6:7:235:LEU:HD23	6:7:357:PRO:HG3	1.84	0.60
6:7:454:ILE:HG23	6:7:595:ASP:OD2	2.02	0.60
2:3:127:LYS:O	2:3:130:THR:OG1	2.19	0.59
2:3:557:ARG:O	2:3:561:ILE:HG12	2.02	0.59
4:5:531:ASP:HA	4:5:534:LYS:HD3	1.84	0.59
3:4:236:LEU:HB3	3:4:238:THR:HG23	1.84	0.59
4:5:31:PHE:CE1	4:5:90:PHE:HE1	2.19	0.59
5:6:778:LYS:HG2	5:6:782:LYS:NZ	2.14	0.59
5:6:794:ARG:H	5:6:795:ILE:HA	1.67	0.59
6:7:470:LEU:HD21	6:7:564:LEU:HD22	1.84	0.59
3:4:666:ASN:HD22	3:4:668:ARG:NH2	1.97	0.59
3:4:682:TYR:O	3:4:691:ASN:ND2	2.35	0.59
5:6:794:ARG:HB2	5:6:796:THR:N	2.16	0.59
6:7:132:ILE:HD13	6:7:144:ASN:HD22	1.67	0.59
6:7:434:LEU:HD21	6:7:699:LEU:HD23	1.84	0.59
2:3:185:ILE:HD13	2:3:291:ARG:HG2	1.84	0.59
3:4:635:ASP:O	3:4:642:ARG:NH2	2.35	0.59
4:5:301:TYR:HE1	4:5:303:SER:HB3	1.67	0.59
4:5:685:GLN:OE1	4:5:688:THR:OG1	2.20	0.59
3:4:315:ARG:NH1	6:7:251:VAL:HG12	2.16	0.59
4:5:197:PHE:CZ	4:5:251:ILE:HD11	2.32	0.59
5:6:109:GLU:O	5:6:112:ARG:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:159:SER:HA	5:6:167:ALA:HB2	1.82	0.59
5:6:752:ARG:C	5:6:756:LYS:HZ3	2.05	0.59
2:3:330:HIS:HD2	2:3:336:VAL:O	1.85	0.59
3:4:231:ASN:O	3:4:234:ARG:HG2	2.02	0.59
3:4:803:ARG:O	3:4:806:GLU:HG2	2.02	0.59
5:6:175:TYR:HA	5:6:178:LEU:HD13	1.85	0.59
5:6:274:HIS:ND1	5:6:288:LEU:HD11	2.18	0.59
5:6:301:ARG:O	5:6:356:TRP:N	2.28	0.59
6:7:486:LYS:N	6:7:487:GLY:HA3	2.17	0.59
2:3:204:ALA:HB1	2:3:205:LYS:HD2	1.84	0.59
3:4:406:VAL:CG2	6:7:560:ARG:HH12	2.15	0.59
5:6:553:GLY:O	5:6:812:ARG:NH1	2.36	0.59
2:3:372:TYR:OH	2:3:561:ILE:O	2.21	0.59
3:4:559:ARG:NE	3:4:668:ARG:HD3	2.17	0.59
3:4:827:ARG:O	3:4:831:SER:N	2.34	0.59
2:3:472:ILE:HG21	2:3:475:PHE:HD1	1.68	0.59
2:3:336:VAL:CG1	2:3:337:ALA:HA	2.33	0.58
2:3:33:ASP:HB2	2:3:39:ARG:HH11	1.68	0.58
2:3:428:LEU:HB3	2:3:429:ALA:HA	1.85	0.58
2:3:672:THR:HG21	2:3:720:THR:HB	1.85	0.58
3:4:833:ILE:HA	3:4:836:TYR:CD2	2.38	0.58
1:2:508:HIS:HB2	1:2:511:ILE:HG22	1.84	0.58
2:3:390:GLU:HB2	2:3:509:ARG:HH22	1.68	0.58
3:4:488:ASN:OD1	3:4:489:LYS:N	2.33	0.58
5:6:808:GLU:O	5:6:812:ARG:HG2	2.03	0.58
1:2:330:VAL:HG23	4:5:272:ARG:HH12	1.68	0.58
2:3:257:THR:HA	2:3:275:ASP:HA	1.85	0.58
3:4:489:LYS:HZ3	3:4:497:GLU:HB2	1.64	0.58
3:4:547:GLY:HA3	3:4:560:GLY:HA2	1.85	0.58
4:5:410:ILE:O	4:5:411:ASN:ND2	2.36	0.58
6:7:113:PHE:O	6:7:117:PHE:HB2	2.03	0.58
6:7:353:GLY:HA3	6:7:377:GLU:O	2.02	0.58
2:3:18:ASP:OD1	2:3:18:ASP:N	2.35	0.58
2:3:194:PRO:HG2	6:7:372:THR:OG1	2.04	0.58
4:5:663:LEU:HG	4:5:666:LEU:HD12	1.86	0.58
2:3:411:PRO:O	2:3:412:SER:OG	2.20	0.58
2:3:493:GLN:HE21	2:3:509:ARG:HA	1.68	0.58
5:6:585:LEU:HD13	5:6:639:ASP:OD1	2.03	0.58
2:3:441:GLY:HA3	2:3:462:MET:HB3	1.85	0.58
3:4:625:ASP:OD1	3:4:668:ARG:HG2	2.04	0.58
6:7:385:LYS:HG2	6:7:639:ARG:NH1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:183:LYS:HA	5:6:186:ARG:HE	1.69	0.58
6:7:440:VAL:HG21	6:7:650:PRO:HD2	1.85	0.58
3:4:517:ASP:O	3:4:520:SER:OG	2.14	0.58
4:5:259:GLN:HE21	4:5:271:PRO:HG2	1.67	0.58
4:5:549:ARG:HA	4:5:651:ARG:HH21	1.68	0.58
4:5:643:ARG:NH1	4:5:692:ALA:HA	2.18	0.58
5:6:385:SER:OG	5:6:457:CYS:O	2.17	0.58
3:4:477:ASP:OD1	3:4:478:THR:N	2.37	0.58
4:5:420:THR:HG23	4:5:556:VAL:HG11	1.85	0.58
5:6:356:TRP:HZ3	5:6:358:LYS:HB2	1.68	0.58
5:6:561:GLU:N	5:6:562:GLY:HA3	2.18	0.58
6:7:214:ARG:CZ	6:7:214:ARG:HB2	2.34	0.57
6:7:584:ILE:HD12	6:7:681:PHE:HZ	1.68	0.57
5:6:359:VAL:HG23	5:6:379:VAL:HG13	1.86	0.57
5:6:820:THR:O	5:6:824:ILE:HG12	2.04	0.57
2:3:362:ILE:HG22	2:3:651:VAL:HG22	1.85	0.57
3:4:243:LEU:HD23	3:4:244:ASP:H	1.69	0.57
1:2:605:LEU:HD23	1:2:647:ILE:HB	1.85	0.57
4:5:621:LYS:O	4:5:624:SER:OG	2.21	0.57
6:7:248:VAL:HG22	6:7:311:GLN:HE21	1.69	0.57
2:3:257:THR:HG22	2:3:275:ASP:HB3	1.87	0.57
5:6:750:GLN:HA	5:6:753:ARG:HH11	1.70	0.57
6:7:541:MET:HB2	6:7:593:ARG:HD3	1.85	0.57
6:7:699:LEU:HB2	6:7:712:ASP:OD1	2.04	0.57
1:2:622:GLU:OE2	1:2:626:GLN:NE2	2.37	0.57
1:2:839:LYS:HZ3	1:2:864:TYR:HA	1.69	0.57
6:7:393:LEU:HD13	6:7:395:SER:HB3	1.86	0.57
3:4:422:GLU:HB3	3:4:494:GLU:OE2	2.04	0.57
1:2:495:ASP:OD1	1:2:509:ARG:NH2	2.35	0.57
2:3:542:ARG:HH12	2:3:700:ARG:NH1	2.01	0.57
3:4:408:ASP:C	3:4:410:GLN:H	2.07	0.57
4:5:572:VAL:HA	4:5:575:ILE:HD12	1.86	0.57
4:5:92:THR:HA	4:5:95:THR:HG22	1.86	0.57
2:3:682:ASN:OD1	2:3:734:ARG:NH1	2.36	0.57
1:2:219:THR:HB	1:2:223:GLY:HA2	1.87	0.57
1:2:688:ASP:HB3	1:2:691:ALA:HB3	1.85	0.57
4:5:259:GLN:NE2	4:5:271:PRO:HG2	2.20	0.57
5:6:283:LYS:O	5:6:286:SER:OG	2.20	0.57
5:6:314:CYS:N	5:6:336:PRO:O	2.38	0.57
1:2:405:HIS:HB2	5:6:621:TYR:CE1	2.40	0.57
6:7:143:LEU:HD22	6:7:199:ARG:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:49:GLN:NE2	4:5:62:THR:OG1	2.37	0.56
4:5:79:LEU:HA	4:5:86:ILE:HD12	1.86	0.56
5:6:566:ARG:HH12	5:6:656:MET:C	2.04	0.56
6:7:86:LEU:CD1	6:7:216:ARG:HG2	2.34	0.56
2:3:291:ARG:HD2	2:3:331:ALA:HB3	1.87	0.56
3:4:502:THR:HG22	3:4:503:ASP:H	1.70	0.56
5:6:273:VAL:HG22	5:6:396:LYS:NZ	2.20	0.56
5:6:270:LEU:HD12	5:6:289:SER:HB2	1.86	0.56
5:6:335:ASN:H	5:6:339:GLU:HA	1.70	0.56
5:6:711:LEU:HG	5:6:712:PHE:H	1.69	0.56
6:7:228:ARG:HH22	6:7:326:HIS:HB3	1.70	0.56
6:7:257:VAL:HG12	6:7:272:GLU:HA	1.86	0.56
2:3:425:THR:HA	2:3:657:ARG:HH11	1.70	0.56
3:4:505:ASP:O	3:4:509:ILE:HD12	2.05	0.56
1:2:686:LEU:HD12	5:6:788:PHE:HZ	1.71	0.56
6:7:411:TYR:CE2	6:7:430:LYS:HE2	2.40	0.56
1:2:235:GLY:HA2	1:2:283:TYR:CE2	2.40	0.56
2:3:547:PHE:HE1	2:3:736:ALA:HB2	1.71	0.56
3:4:239:SER:OG	3:4:240:ASN:N	2.38	0.56
3:4:527:ALA:HB3	3:4:537:LYS:HZ2	1.69	0.56
4:5:148:LEU:HD23	4:5:260:GLU:HB3	1.87	0.56
5:6:297:THR:HA	5:6:359:VAL:HG12	1.88	0.56
1:2:557:GLU:OE2	1:2:565:PHE:CD1	2.59	0.56
4:5:421:ALA:HA	7:5:2001:ADP:H5'2	1.86	0.56
3:4:349:CYS:N	3:4:353:ASP:OD1	2.34	0.56
6:7:182:ARG:O	6:7:186:GLU:HG2	2.04	0.56
1:2:855:ARG:HG3	1:2:858:ARG:HH21	1.70	0.56
5:6:344:TRP:CB	5:6:345:THR:HA	2.36	0.56
2:3:284:ASP:OD1	6:7:329:ARG:NH2	2.39	0.56
4:5:464:LEU:HD11	4:5:470:VAL:HG21	1.87	0.56
1:2:339:PHE:HE1	1:2:375:VAL:HG22	1.71	0.56
2:3:367:LEU:HD12	2:3:378:LYS:HB3	1.88	0.56
3:4:764:GLU:HA	3:4:767:LYS:HZ1	1.67	0.56
2:3:399:LEU:HD22	6:7:620:HIS:CE1	2.41	0.56
1:2:212:LYS:HZ1	1:2:275:ALA:HB2	1.71	0.56
1:2:290:HIS:O	1:2:292:GLU:N	2.38	0.56
1:2:323:VAL:HG22	1:2:423:GLU:HG3	1.87	0.56
1:2:506:TYR:OH	1:2:694:ARG:HD3	2.05	0.56
3:4:447:ASN:O	3:4:448:SER:OG	2.22	0.56
3:4:569:ASP:O	3:4:572:THR:OG1	2.19	0.56
1:2:308:GLU:OE1	1:2:310:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:580:VAL:HG21	1:2:636:ILE:HG21	1.88	0.56
6:7:208:SER:HB3	6:7:209:GLN:HG3	1.88	0.56
6:7:401:VAL:HG13	6:7:641:TYR:HD1	1.71	0.56
1:2:229:ALA:HA	1:2:232:ARG:HG2	1.87	0.55
2:3:475:PHE:HB3	2:3:516:ALA:HB2	1.87	0.55
3:4:764:GLU:HA	3:4:767:LYS:HZ3	1.68	0.55
1:2:689:GLU:OE2	5:6:778:LYS:HD3	2.06	0.55
6:7:281:LEU:HD12	6:7:298:LEU:HD11	1.88	0.55
6:7:601:LEU:HD21	6:7:727:LEU:HA	1.88	0.55
1:2:296:ARG:O	1:2:455:SER:OG	2.24	0.55
2:3:202:TYR:HD1	2:3:209:PHE:CE1	2.25	0.55
3:4:428:ARG:CZ	3:4:485:LEU:HD12	2.36	0.55
3:4:527:ALA:HB1	3:4:530:ILE:HD13	1.86	0.55
5:6:134:LYS:N	5:6:135:VAL:HA	2.21	0.55
5:6:791:SER:OG	5:6:839:ASP:OD1	2.17	0.55
3:4:646:HIS:HA	3:4:701:ARG:NH1	2.21	0.55
5:6:143:MET:HE2	5:6:150:THR:H	1.71	0.55
5:6:543:VAL:HG21	5:6:715:ILE:HD11	1.88	0.55
2:3:362:ILE:HG22	2:3:651:VAL:CG2	2.35	0.55
2:3:493:GLN:HE21	2:3:509:ARG:CA	2.19	0.55
1:2:808:ARG:HG2	7:5:2001:ADP:H4'	1.88	0.55
4:5:409:ASP:OD1	4:5:410:ILE:HG12	2.06	0.55
4:5:437:VAL:HG12	4:5:439:THR:HG23	1.87	0.55
5:6:356:TRP:CZ3	5:6:358:LYS:HB2	2.41	0.55
5:6:776:LYS:HG3	5:6:779:GLU:OE2	2.07	0.55
6:7:421:GLU:HA	6:7:625:GLN:HE22	1.72	0.55
2:3:346:ASP:HA	2:3:349:ASN:HD22	1.72	0.55
2:3:558:ASP:OD2	4:5:627:VAL:HA	2.05	0.55
3:4:345:ALA:O	3:4:357:ALA:HB1	2.06	0.55
3:4:370:ARG:HH22	5:6:426:ILE:HG13	1.71	0.55
1:2:410:LEU:HD22	1:2:456:ILE:HD11	1.87	0.55
2:3:375:ASP:O	2:3:379:LYS:HG3	2.06	0.55
2:3:655:PHE:HA	2:3:658:LYS:NZ	2.21	0.55
2:3:690:ASP:HA	2:3:693:LYS:HB2	1.89	0.55
4:5:86:ILE:O	4:5:89:LEU:N	2.39	0.55
6:7:661:VAL:O	6:7:665:ILE:HD12	2.07	0.55
2:3:706:ILE:HD13	6:7:620:HIS:HD2	1.72	0.55
4:5:35:ILE:HD11	4:5:94:ILE:HG13	1.89	0.55
5:6:115:PHE:O	5:6:118:PHE:HB3	2.07	0.55
6:7:214:ARG:CG	6:7:215:TYR:O	2.54	0.55
3:4:400:GLN:HE22	6:7:555:THR:HA	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:132:VAL:HG22	5:6:133:GLU:OE1	2.06	0.55
5:6:534:ALA:HB3	5:6:544:LYS:HE2	1.88	0.55
6:7:441:ASP:OD1	6:7:442:LYS:N	2.40	0.55
1:2:484:PHE:CE1	1:2:766:TYR:HD1	2.25	0.55
1:2:560:ALA:HB3	1:2:563:ALA:HB2	1.89	0.55
2:3:678:VAL:HG21	2:3:723:LYS:HG3	1.87	0.55
3:4:331:LEU:HA	3:4:431:ASP:O	2.07	0.55
4:5:675:ARG:HG3	4:5:676:HIS:N	2.21	0.55
5:6:158:LEU:HD21	5:6:170:ILE:HD12	1.88	0.55
6:7:165:ASN:HB3	6:7:166:LEU:CA	2.37	0.55
6:7:426:LEU:O	6:7:430:LYS:HB2	2.07	0.55
1:2:601:LYS:NZ	1:2:643:ARG:HH11	2.04	0.55
2:3:389:VAL:HG12	2:3:390:GLU:N	2.14	0.55
5:6:696:ARG:O	5:6:696:ARG:NH1	2.36	0.55
6:7:90:ASN:HD21	6:7:214:ARG:NE	2.03	0.55
1:2:793:LEU:HD21	1:2:842:VAL:HG22	1.89	0.54
2:3:653:ILE:HD12	4:5:402:ASP:HA	1.88	0.54
4:5:90:PHE:CD2	4:5:137:LEU:HD21	2.42	0.54
4:5:49:GLN:O	4:5:53:ASN:ND2	2.40	0.54
4:5:376:PRO:HB2	4:5:585:ASN:HD21	1.73	0.54
6:7:1:MET:HG2	6:7:2:SER:O	2.06	0.54
6:7:462:PRO:HD3	6:7:573:ARG:HE	1.72	0.54
3:4:455:SER:OG	3:4:456:LEU:N	2.35	0.54
3:4:651:GLN:HE21	5:6:586:LYS:HZ3	1.54	0.54
3:4:565:LEU:HB2	3:4:702:PHE:CD2	2.42	0.54
1:2:264:PRO:HG3	1:2:317:LEU:HB2	1.89	0.54
5:6:575:GLY:C	5:6:581:LYS:HZ1	2.06	0.54
5:6:601:LYS:HB2	5:6:643:LYS:HB3	1.90	0.54
6:7:90:ASN:HD21	6:7:214:ARG:HE	1.56	0.54
4:5:631:LYS:HE3	4:5:635:ILE:HD11	1.88	0.54
5:6:517:LYS:O	5:6:521:LYS:HG2	2.07	0.54
6:7:398:GLU:O	6:7:402:MET:HG3	2.08	0.54
6:7:421:GLU:HA	6:7:625:GLN:NE2	2.23	0.54
1:2:557:GLU:OE2	1:2:565:PHE:HB2	2.07	0.54
2:3:332:ARG:O	2:3:333:SER:OG	2.21	0.54
2:3:354:SER:HB3	2:3:717:LEU:HD22	1.89	0.54
5:6:183:LYS:HZ1	5:6:186:ARG:HH12	1.53	0.54
2:3:169:ARG:NH2	2:3:269:GLN:OE1	2.40	0.54
6:7:208:SER:CB	6:7:209:GLN:CA	2.85	0.54
3:4:604:TYR:OH	6:7:554:ASN:OD1	2.23	0.54
6:7:87:GLN:NE2	6:7:214:ARG:NH1	2.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:212:LYS:NZ	1:2:275:ALA:HB2	2.23	0.54
2:3:687:ARG:HH12	2:3:698:THR:HA	1.73	0.54
4:5:441:GLY:HA3	4:5:443:GLY:H	1.73	0.54
5:6:781:ARG:NE	5:6:795:ILE:O	2.41	0.54
6:7:443:ARG:NH1	6:7:449:LYS:HZ2	2.06	0.54
1:2:234:LEU:HD12	1:2:234:LEU:O	2.08	0.54
2:3:32:LEU:HD11	2:3:132:LEU:HD22	1.89	0.54
2:3:362:ILE:HG23	2:3:651:VAL:HG21	1.88	0.54
3:4:545:PHE:CE1	3:4:751:ILE:HG12	2.43	0.54
3:4:408:ASP:OD1	6:7:517:ASP:OD2	2.25	0.54
1:2:429:ILE:HD12	1:2:431:LYS:HE2	1.90	0.54
2:3:440:VAL:HG12	2:3:441:GLY:H	1.73	0.54
2:3:712:HIS:ND1	2:3:725:ASP:OD1	2.38	0.54
4:5:569:ALA:O	4:5:573:ILE:HD12	2.08	0.54
5:6:112:ARG:HH22	5:6:183:LYS:HB2	1.73	0.54
1:2:230:ARG:O	1:2:233:THR:OG1	2.24	0.53
1:2:517:CYS:SG	1:2:816:ILE:HG23	2.49	0.53
3:4:572:THR:O	3:4:573:SER:OG	2.18	0.53
2:3:553:ILE:HB	4:5:630:ARG:HH11	1.72	0.53
4:5:545:THR:O	4:5:548:SER:OG	2.19	0.53
4:5:685:GLN:O	4:5:688:THR:OG1	2.27	0.53
6:7:459:MET:HG3	6:7:460:GLY:H	1.73	0.53
1:2:297:ILE:HG22	1:2:298:SER:N	2.20	0.53
4:5:621:LYS:HG2	4:5:674:GLU:OE2	2.08	0.53
4:5:65:MET:HG2	4:5:76:TYR:HE1	1.74	0.53
5:6:663:ILE:HD12	5:6:672:LEU:HD12	1.90	0.53
6:7:493:LEU:HD12	6:7:494:THR:N	2.24	0.53
3:4:253:GLN:O	3:4:254:THR:OG1	2.19	0.53
3:4:366:GLN:N	3:4:366:GLN:OE1	2.42	0.53
5:6:603:SER:N	5:6:604:SER:HA	2.24	0.53
6:7:138:VAL:HG21	6:7:303:ARG:NH2	2.23	0.53
6:7:459:MET:HB3	6:7:599:LEU:HA	1.90	0.53
2:3:171:LEU:HD23	2:3:172:THR:N	2.23	0.53
4:5:577:THR:OG1	4:5:578:GLY:HA2	2.07	0.53
2:3:561:ILE:HG21	4:5:650:ILE:HG21	1.89	0.53
5:6:136:TYR:O	5:6:140:ILE:HD12	2.09	0.53
5:6:183:LYS:HA	5:6:186:ARG:NE	2.23	0.53
6:7:570:LEU:HD13	6:7:585:ASN:HD21	1.73	0.53
1:2:387:ARG:HD2	1:2:407:GLU:OE2	2.09	0.53
5:6:529:LEU:O	5:6:533:ILE:HG13	2.09	0.53
5:6:776:LYS:NZ	5:6:824:ILE:HG22	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:223:LYS:O	6:7:225:LEU:HG	2.09	0.53
6:7:404:LEU:HD11	6:7:414:LEU:HD21	1.91	0.53
1:2:809:HIS:HE1	1:2:845:PHE:HB2	1.74	0.53
2:3:25:VAL:HG13	2:3:128:ALA:HB2	1.91	0.53
2:3:690:ASP:O	2:3:694:LYS:N	2.40	0.53
5:6:305:TYR:CD1	5:6:306:LYS:HG2	2.43	0.53
5:6:780:LEU:HD12	5:6:828:TYR:CE1	2.43	0.53
2:3:100:LEU:HB3	2:3:111:TRP:CZ3	2.43	0.53
4:5:409:ASP:OD1	4:5:410:ILE:HG23	2.09	0.53
5:6:117:GLN:HG2	5:6:121:ASP:OD2	2.09	0.53
5:6:611:ALA:N	5:6:624:GLU:OE2	2.41	0.53
6:7:484:THR:O	6:7:488:SER:N	2.26	0.53
6:7:536:ALA:O	6:7:540:VAL:HG23	2.08	0.53
2:3:221:LEU:HD11	2:3:297:VAL:HG21	1.91	0.52
4:5:543:GLN:HE21	4:5:546:ILE:HD11	1.73	0.52
5:6:448:LEU:HD12	5:6:448:LEU:O	2.09	0.52
6:7:137:ASP:OD1	6:7:138:VAL:N	2.42	0.52
3:4:488:ASN:O	3:4:489:LYS:HB3	2.09	0.52
5:6:151:ILE:HD11	5:6:265:ILE:HG23	1.91	0.52
6:7:538:HIS:HD2	6:7:593:ARG:HE	1.56	0.52
6:7:664:TYR:HB2	6:7:689:LEU:HD13	1.90	0.52
2:3:429:ALA:HB3	2:3:469:VAL:O	2.09	0.52
3:4:408:ASP:HB2	6:7:560:ARG:NH2	2.24	0.52
4:5:601:ARG:O	4:5:604:THR:OG1	2.27	0.52
5:6:142:PHE:HA	5:6:145:ILE:HG12	1.91	0.52
6:7:132:ILE:HD13	6:7:144:ASN:ND2	2.24	0.52
1:2:790:TYR:CG	1:2:810:LEU:HD12	2.45	0.52
4:5:31:PHE:CE1	4:5:75:ILE:HG21	2.44	0.52
6:7:541:MET:HB2	6:7:593:ARG:HH11	1.75	0.52
1:2:294:HIS:HD2	1:2:296:ARG:HH12	1.58	0.52
1:2:339:PHE:CE1	1:2:375:VAL:HG22	2.45	0.52
1:2:795:ARG:HA	1:2:798:ILE:HD12	1.90	0.52
2:3:443:THR:HB	2:3:457:LEU:HB3	1.90	0.52
3:4:598:ALA:HB1	5:6:601:LYS:HZ1	1.75	0.52
4:5:66:GLU:OE2	4:5:143:ALA:HB2	2.09	0.52
4:5:90:PHE:O	4:5:94:ILE:HD12	2.09	0.52
5:6:116:GLU:OE2	5:6:187:ARG:HD3	2.10	0.52
2:3:199:SER:HB3	2:3:212:ARG:HB3	1.92	0.52
2:3:466:ASP:OD1	2:3:467:ARG:N	2.43	0.52
3:4:437:GLY:HA3	3:4:463:VAL:HA	1.92	0.52
3:4:417:LEU:HD13	3:4:463:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:658:LYS:HB3	5:6:604:SER:N	2.24	0.52
4:5:19:PRO:HG2	4:5:21:ASP:HB2	1.90	0.52
4:5:678:ASP:O	4:5:682:ARG:NH1	2.42	0.52
5:6:335:ASN:N	5:6:339:GLU:HA	2.24	0.52
5:6:558:SER:CB	5:6:559:THR:HA	2.33	0.52
6:7:214:ARG:HG2	6:7:216:ARG:HB2	1.92	0.52
6:7:90:ASN:HD22	6:7:214:ARG:NH1	2.08	0.52
2:3:422:VAL:O	2:3:426:ALA:HB2	2.10	0.52
2:3:476:ASP:OD1	2:3:477:LYS:N	2.43	0.52
3:4:568:GLY:N	3:4:574:LYS:HZ3	2.08	0.52
4:5:655:ALA:O	4:5:659:ILE:HD12	2.10	0.52
1:2:805:ILE:H	1:2:805:ILE:HD12	1.74	0.52
4:5:282:LEU:HD22	4:5:333:ILE:HG22	1.92	0.52
5:6:264:GLN:NE2	5:6:383:GLY:HA2	2.25	0.52
5:6:763:PRO:HG3	5:6:812:ARG:HD3	1.92	0.52
6:7:135:LYS:HA	6:7:136:ASP:HB3	1.91	0.52
2:3:183:GLU:OE1	2:3:183:GLU:N	2.43	0.52
3:4:443:PRO:HB3	3:4:457:TYR:CE1	2.45	0.52
4:5:349:PHE:HZ	4:5:609:LYS:HZ1	1.55	0.52
4:5:396:SER:HB3	4:5:661:GLU:HG2	1.91	0.52
5:6:804:ILE:O	5:6:807:SER:OG	2.21	0.52
3:4:280:MET:O	3:4:284:ILE:HD12	2.10	0.52
3:4:657:ALA:HA	3:4:662:ILE:HG23	1.91	0.52
6:7:244:ILE:HD12	6:7:318:LEU:HA	1.92	0.52
2:3:193:ARG:HD2	6:7:371:LEU:HD23	1.91	0.52
1:2:481:GLU:O	1:2:485:ARG:HG2	2.10	0.51
1:2:527:VAL:O	1:2:530:LYS:N	2.43	0.51
2:3:450:ARG:HH12	4:5:460:ARG:HB2	1.75	0.51
3:4:190:CYS:SG	3:4:257:LEU:HD13	2.50	0.51
4:5:379:PHE:H	7:5:2001:ADP:N6	2.06	0.51
4:5:498:GLU:N	4:5:498:GLU:OE1	2.42	0.51
2:3:187:THR:O	2:3:257:THR:OG1	2.28	0.51
3:4:313:GLY:HA2	3:4:403:PRO:HB3	1.92	0.51
4:5:172:LEU:HD22	4:5:252:ASP:OD2	2.09	0.51
1:2:856:GLN:NE2	1:2:859:ARG:HH21	2.08	0.51
5:6:615:ASP:OD2	5:6:617:GLU:HA	2.10	0.51
1:2:211:LEU:HA	1:2:214:PHE:HB3	1.93	0.51
1:2:343:LYS:HZ3	1:2:371:GLY:HA2	1.76	0.51
2:3:397:SER:HB2	6:7:471:LYS:HD2	1.92	0.51
6:7:197:THR:O	6:7:198:ARG:HD2	2.11	0.51
6:7:90:ASN:ND2	6:7:214:ARG:HE	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:723:SER:OG	6:7:724:LYS:N	2.43	0.51
1:2:335:LYS:HD2	1:2:383:ARG:HH11	1.76	0.51
1:2:434:TYR:CG	1:2:435:ASP:N	2.79	0.51
1:2:446:VAL:HG21	5:6:356:TRP:HZ2	1.75	0.51
2:3:491:GLU:CD	2:3:700:ARG:HH22	2.14	0.51
3:4:491:ASP:OD1	3:4:492:HIS:N	2.42	0.51
4:5:608:LEU:HD11	4:5:609:LYS:HZ3	1.72	0.51
4:5:87:ILE:O	4:5:90:PHE:HB2	2.11	0.51
5:6:580:SER:HA	7:6:2001:ADP:H5'2	1.91	0.51
5:6:540:HIS:C	5:6:542:ALA:H	2.13	0.51
1:2:286:TYR:CE2	1:2:293:ILE:HD11	2.45	0.51
1:2:562:ARG:HH22	4:5:265:VAL:HG13	1.74	0.51
5:6:400:VAL:O	5:6:455:LEU:HB3	2.11	0.51
1:2:689:GLU:OE1	5:6:782:LYS:HD3	2.09	0.51
4:5:44:PHE:CE1	4:5:47:ARG:HD3	2.45	0.51
2:3:430:ILE:HG12	4:5:510:THR:HG21	1.91	0.51
6:7:208:SER:CB	6:7:209:GLN:CB	2.83	0.51
6:7:667:LEU:O	6:7:670:ASP:OD1	2.29	0.51
1:2:520:PHE:CD1	1:2:767:ILE:HG22	2.46	0.51
1:2:601:LYS:HZ1	1:2:643:ARG:HD2	1.75	0.51
1:2:790:TYR:CD1	1:2:810:LEU:HD12	2.46	0.51
3:4:411:THR:OG1	3:4:412:PRO:HD2	2.11	0.51
4:5:2:SER:OG	4:5:3:PHE:N	2.43	0.51
6:7:114:THR:HG22	6:7:204:PHE:HE2	1.75	0.51
6:7:446:ASP:HB2	6:7:447:GLY:HA2	1.92	0.51
6:7:456:VAL:HB	6:7:564:LEU:HG	1.93	0.51
6:7:619:VAL:HG22	6:7:622:HIS:O	2.11	0.51
2:3:103:LEU:O	2:3:107:ASP:N	2.44	0.51
2:3:403:ILE:HD11	2:3:707:ARG:HB3	1.93	0.51
3:4:458:LYS:HZ1	5:6:413:PRO:HB3	1.75	0.51
5:6:412:LEU:HB3	5:6:416:LYS:HZ1	1.75	0.51
1:2:215:LEU:HD21	1:2:231:ILE:HD11	1.92	0.51
4:5:607:ARG:HA	4:5:665:LYS:CE	2.42	0.51
6:7:656:VAL:O	6:7:660:VAL:HG23	2.11	0.51
1:2:215:LEU:HD12	1:2:227:TYR:HB3	1.92	0.50
1:2:846:VAL:O	1:2:853:VAL:HG21	2.12	0.50
3:4:231:ASN:HA	3:4:234:ARG:HG2	1.93	0.50
6:7:127:LEU:HG	6:7:128:PRO:HD3	1.93	0.50
6:7:90:ASN:HD22	6:7:214:ARG:HH11	1.60	0.50
1:2:486:LYS:O	1:2:489:ARG:HG2	2.11	0.50
4:5:138:ILE:HG23	4:5:332:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:31:PHE:CZ	4:5:90:PHE:HE1	2.29	0.50
5:6:691:ARG:HH11	5:6:716:LEU:CD2	2.17	0.50
2:3:209:PHE:CE2	6:7:10:LEU:HD12	2.47	0.50
6:7:400:ARG:HB3	6:7:637:LYS:NZ	2.26	0.50
2:3:374:HIS:HE1	2:3:549:VAL:HG11	1.76	0.50
2:3:33:ASP:HB2	2:3:39:ARG:NH1	2.26	0.50
2:3:372:TYR:CE2	2:3:561:ILE:HG23	2.46	0.50
2:3:704:THR:HA	2:3:707:ARG:HH11	1.77	0.50
3:4:362:ARG:HH11	6:7:299:PHE:HZ	1.59	0.50
4:5:180:SER:OG	4:5:247:SER:OG	2.18	0.50
4:5:629:ILE:HG23	4:5:633:LEU:HD12	1.93	0.50
6:7:440:VAL:O	6:7:441:ASP:OD1	2.28	0.50
1:2:211:LEU:O	1:2:214:PHE:HB3	2.11	0.50
1:2:212:LYS:HG3	1:2:274:VAL:HG12	1.92	0.50
2:3:171:LEU:HD23	2:3:172:THR:H	1.76	0.50
2:3:652:THR:CB	2:3:654:PRO:HD3	2.40	0.50
4:5:256:LEU:HB2	4:5:276:MET:HB2	1.92	0.50
5:6:393:ASP:OD1	5:6:394:ARG:N	2.45	0.50
5:6:401:GLU:OE2	5:6:452:ILE:HG23	2.10	0.50
6:7:689:LEU:O	6:7:692:ILE:HG22	2.11	0.50
2:3:651:VAL:O	2:3:651:VAL:CG1	2.59	0.50
4:5:208:PRO:HG2	4:5:241:TYR:CD2	2.47	0.50
1:2:335:LYS:HD2	1:2:383:ARG:NH1	2.26	0.50
1:2:815:ARG:O	1:2:818:GLU:HG2	2.11	0.50
2:3:372:TYR:OH	2:3:564:HIS:HB3	2.12	0.50
3:4:403:PRO:O	3:4:404:ASP:OD1	2.29	0.50
5:6:777:TYR:CE1	5:6:800:LEU:HB2	2.47	0.50
6:7:396:ASP:O	6:7:399:GLU:HB3	2.11	0.50
1:2:621:HIS:NE2	4:5:481:GLU:OE2	2.44	0.50
2:3:389:VAL:H	2:3:714:LYS:NZ	2.10	0.50
2:3:669:PRO:HG2	2:3:710:THR:HG23	1.93	0.50
3:4:306:TYR:CD2	3:4:307:ASN:HB2	2.46	0.50
3:4:545:PHE:HE1	3:4:751:ILE:HG23	1.77	0.50
3:4:769:GLU:HA	3:4:772:ARG:HG2	1.93	0.50
4:5:69:ILE:HD12	4:5:73:GLU:HA	1.94	0.50
5:6:183:LYS:CB	5:6:186:ARG:HH11	2.25	0.50
6:7:409:ASP:OD2	6:7:412:ASN:HB3	2.12	0.50
1:2:444:PHE:O	1:2:446:VAL:HG23	2.11	0.50
2:3:163:ALA:HB3	2:3:164:HIS:ND1	2.25	0.50
2:3:189:THR:HG22	2:3:190:SER:N	2.27	0.50
2:3:683:TYR:CZ	2:3:687:ARG:HD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:793:TYR:O	5:6:794:ARG:NH1	2.40	0.50
2:3:451:GLU:O	2:3:452:THR:OG1	2.25	0.50
3:4:428:ARG:HH11	3:4:482:GLU:HA	1.77	0.50
3:4:534:GLU:N	3:4:534:GLU:OE1	2.38	0.50
3:4:677:PRO:HG2	3:4:680:SER:O	2.12	0.50
4:5:254:GLN:HG2	4:5:256:LEU:HD12	1.94	0.50
4:5:340:SER:HB2	4:5:342:ILE:HG13	1.94	0.50
4:5:481:GLU:HB3	4:5:484:LYS:HB2	1.94	0.50
5:6:775:GLU:HA	5:6:778:LYS:HB3	1.93	0.50
6:7:333:ILE:HG12	6:7:376:LEU:HB3	1.94	0.50
1:2:335:LYS:CD	1:2:383:ARG:HH11	2.25	0.49
3:4:299:LYS:NZ	3:4:301:TYR:HE1	2.10	0.49
3:4:354:HIS:HB2	3:4:373:ARG:HB2	1.93	0.49
3:4:732:LYS:HD2	3:4:733:PRO:HD2	1.94	0.49
4:5:141:SER:H	4:5:295:VAL:HG21	1.77	0.49
4:5:45:ILE:HG13	4:5:46:TYR:N	2.27	0.49
5:6:653:HIS:NE2	5:6:704:PRO:HB2	2.27	0.49
1:2:332:PRO:HG3	4:5:300:ILE:HD11	1.94	0.49
5:6:118:PHE:HD1	5:6:161:ARG:HD3	1.77	0.49
6:7:149:ARG:HH11	6:7:152:ARG:NE	2.10	0.49
2:3:252:ASP:OD2	6:7:231:LYS:NZ	2.45	0.49
1:2:585:ILE:HG12	1:2:586:THR:H	1.77	0.49
2:3:126:GLU:O	2:3:130:THR:HG23	2.13	0.49
2:3:414:ALA:O	2:3:418:LEU:N	2.41	0.49
2:3:652:THR:CA	2:3:654:PRO:HD3	2.38	0.49
3:4:324:LYS:NZ	6:7:138:VAL:HG11	2.27	0.49
1:2:546:GLY:HA3	5:6:796:THR:HG23	1.93	0.49
6:7:458:LEU:HD23	6:7:598:PHE:HB2	1.94	0.49
3:4:354:HIS:NE2	3:4:356:MET:HG2	2.26	0.49
4:5:407:ARG:O	4:5:658:ARG:HD3	2.13	0.49
4:5:677:VAL:O	4:5:681:ILE:HD12	2.11	0.49
7:6:2001:ADP:H2'	7:6:2001:ADP:N3	2.26	0.49
1:2:853:VAL:O	1:2:856:GLN:HB3	2.12	0.49
2:3:195:LYS:HA	6:7:371:LEU:HA	1.94	0.49
3:4:315:ARG:HG2	3:4:410:GLN:NE2	2.28	0.49
3:4:378:GLU:O	3:4:380:ASN:N	2.41	0.49
4:5:338:GLU:N	4:5:339:THR:HA	2.28	0.49
4:5:413:LEU:HD11	4:5:550:PHE:CD2	2.47	0.49
7:3:2001:ADP:O5'	4:5:651:ARG:NH1	2.45	0.49
5:6:380:ILE:O	5:6:455:LEU:HD12	2.13	0.49
6:7:232:GLY:O	6:7:235:LEU:HD13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:636:SER:HA	6:7:639:ARG:HH21	1.77	0.49
1:2:384:ASN:OD1	1:2:384:ASN:N	2.45	0.49
1:2:481:GLU:HA	1:2:484:PHE:HB3	1.93	0.49
1:2:693:GLU:CA	5:6:778:LYS:HZ1	2.25	0.49
3:4:419:VAL:HA	3:4:463:VAL:HG23	1.94	0.49
5:6:273:VAL:HG22	5:6:396:LYS:HZ1	1.77	0.49
6:7:240:THR:HG23	6:7:352:THR:HG22	1.93	0.49
1:2:247:ARG:NH2	1:2:299:ASP:OD2	2.45	0.49
1:2:274:VAL:HA	1:2:277:GLU:HG2	1.94	0.49
2:3:480:ASP:O	2:3:484:VAL:HG23	2.13	0.49
4:5:4:ASP:OD1	4:5:4:ASP:N	2.43	0.49
3:4:658:LYS:CB	5:6:604:SER:H	2.26	0.49
6:7:90:ASN:ND2	6:7:214:ARG:NE	2.60	0.49
6:7:235:LEU:HD12	6:7:355:PHE:HE2	1.77	0.49
6:7:436:LEU:HD21	6:7:473:ILE:HG23	1.93	0.49
3:4:188:GLN:C	3:4:190:CYS:N	2.64	0.49
3:4:244:ASP:OD2	3:4:247:ASN:ND2	2.45	0.49
5:6:547:ILE:HD11	5:6:584:PHE:HB3	1.94	0.49
5:6:701:MET:HB2	5:6:705:ILE:HD11	1.94	0.49
1:2:840:VAL:O	1:2:843:ASP:OD1	2.31	0.49
3:4:184:ASN:HD22	6:7:141:VAL:HG11	1.78	0.49
3:4:585:THR:HG21	3:4:628:VAL:H	1.78	0.49
6:7:28:PHE:HE2	6:7:31:ASP:H	1.60	0.49
3:4:408:ASP:OD2	6:7:517:ASP:OD1	2.30	0.49
1:2:220:ASP:OD1	1:2:221:GLU:N	2.44	0.49
1:2:597:VAL:HG23	1:2:629:ILE:HD12	1.94	0.49
2:3:101:ASP:OD1	2:3:104:ARG:NH2	2.46	0.49
3:4:521:LEU:O	3:4:524:ARG:HG2	2.13	0.49
3:4:635:ASP:OD2	3:4:675:ALA:HB1	2.13	0.49
5:6:780:LEU:HD12	5:6:828:TYR:HE1	1.78	0.49
6:7:397:VAL:HA	6:7:400:ARG:HH21	1.77	0.49
1:2:518:SER:OG	1:2:537:ILE:O	2.23	0.48
1:2:811:GLU:OE1	1:2:815:ARG:NH1	2.45	0.48
2:3:406:LEU:HB3	2:3:546:LEU:HD23	1.94	0.48
2:3:653:ILE:HD13	4:5:402:ASP:HA	1.83	0.48
3:4:367:GLU:OE1	3:4:367:GLU:N	2.43	0.48
5:6:603:SER:H	5:6:604:SER:HA	1.78	0.48
6:7:322:VAL:HG12	6:7:323:PRO:O	2.13	0.48
6:7:443:ARG:NH1	6:7:449:LYS:HZ1	2.02	0.48
6:7:89:GLN:NE2	6:7:102:LEU:H	2.11	0.48
1:2:230:ARG:NH1	1:2:243:GLU:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:566:LEU:HD13	4:5:619:ALA:HB1	1.94	0.48
3:4:527:ALA:HB3	3:4:537:LYS:HZ3	1.79	0.48
3:4:821:ASP:OD1	3:4:821:ASP:C	2.51	0.48
4:5:464:LEU:HD12	4:5:513:LEU:HD22	1.95	0.48
5:6:601:LYS:HA	5:6:644:MET:HG2	1.96	0.48
5:6:778:LYS:C	5:6:782:LYS:NZ	2.67	0.48
6:7:394:THR:HG23	6:7:398:GLU:OE2	2.13	0.48
2:3:435:ARG:NH1	2:3:477:LYS:O	2.45	0.48
6:7:128:PRO:HD2	6:7:129:THR:HA	1.95	0.48
6:7:220:ILE:HA	6:7:223:LYS:HZ1	1.76	0.48
2:3:427:SER:O	2:3:428:LEU:HB2	2.13	0.48
4:5:211:CYS:HB2	4:5:240:PRO:HG3	1.94	0.48
4:5:28:ILE:HG23	4:5:93:ALA:HB2	1.95	0.48
4:5:349:PHE:CZ	4:5:609:LYS:NZ	2.80	0.48
6:7:334:HIS:HD2	6:7:375:TYR:CD1	2.31	0.48
6:7:459:MET:HG3	6:7:569:PRO:HG3	1.95	0.48
1:2:684:ARG:HB3	1:2:685:ASP:CA	2.43	0.48
1:2:767:ILE:HG13	1:2:768:HIS:N	2.29	0.48
3:4:505:ASP:OD1	3:4:505:ASP:N	2.46	0.48
3:4:587:ARG:HD2	3:4:625:ASP:O	2.13	0.48
4:5:342:ILE:HG22	4:5:345:SER:HB3	1.95	0.48
5:6:597:TYR:HD1	5:6:637:CYS:SG	2.37	0.48
6:7:133:ASP:CG	6:7:134:TYR:H	2.16	0.48
6:7:421:GLU:C	6:7:625:GLN:HE22	2.16	0.48
3:4:309:GLY:O	3:4:327:ASN:ND2	2.46	0.48
3:4:306:TYR:HB3	3:4:465:HIS:CD2	2.49	0.48
5:6:134:LYS:HZ3	5:6:137:ARG:HD2	1.78	0.48
6:7:441:ASP:HB3	6:7:452:GLY:HA2	1.95	0.48
1:2:405:HIS:ND1	5:6:621:TYR:HB2	2.29	0.48
4:5:331:LEU:HD12	4:5:331:LEU:O	2.14	0.48
6:7:214:ARG:CB	6:7:214:ARG:HH21	2.24	0.48
3:4:445:ARG:HG2	3:4:453:LEU:HD23	1.95	0.48
6:7:198:ARG:O	6:7:199:ARG:HB3	2.14	0.48
3:4:243:LEU:HD23	3:4:244:ASP:N	2.29	0.48
3:4:497:GLU:HG3	3:4:498:VAL:N	2.28	0.48
3:4:600:GLY:HA2	3:4:604:TYR:HE1	1.77	0.48
4:5:489:ASP:O	4:5:493:ILE:HG12	2.14	0.48
3:4:625:ASP:HB3	5:6:370:THR:OG1	2.14	0.48
3:4:340:PRO:HD3	5:6:452:ILE:HD12	1.95	0.48
6:7:395:SER:C	6:7:397:VAL:H	2.16	0.48
6:7:460:GLY:HA3	6:7:600:MET:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:570:LEU:HB2	6:7:585:ASN:HD21	1.79	0.48
6:7:584:ILE:HD12	6:7:681:PHE:CZ	2.48	0.48
1:2:601:LYS:HZ1	1:2:643:ARG:NH1	2.11	0.48
2:3:189:THR:HA	2:3:256:ILE:HG22	1.95	0.48
2:3:198:ARG:O	2:3:248:SER:HB2	2.14	0.48
4:5:357:PHE:HE1	4:5:598:LYS:HE2	1.78	0.48
4:5:38:PHE:HZ	4:5:67:HIS:NE2	2.11	0.48
1:2:340:ASN:HD21	1:2:374:ARG:NH2	2.12	0.47
1:2:405:HIS:CE1	5:6:621:TYR:HB2	2.48	0.47
2:3:653:ILE:HD13	4:5:402:ASP:HB2	1.74	0.47
3:4:177:LEU:HD12	3:4:178:ARG:O	2.14	0.47
3:4:443:PRO:HB3	3:4:457:TYR:HE1	1.77	0.47
3:4:563:ASN:HD22	3:4:649:MET:CE	2.27	0.47
2:3:390:GLU:HG2	2:3:509:ARG:NH1	2.29	0.47
3:4:796:ARG:NH1	7:6:2001:ADP:H4'	2.29	0.47
4:5:19:PRO:N	4:5:20:ASN:HA	2.29	0.47
3:4:318:ASN:HD22	6:7:341:ARG:HH12	1.63	0.47
2:3:346:ASP:O	2:3:350:ILE:HD12	2.14	0.47
2:3:372:TYR:H	7:3:2001:ADP:HN62	1.62	0.47
2:3:447:THR:HB	2:3:448:THR:HG22	1.95	0.47
4:5:299:SER:OG	4:5:300:ILE:N	2.48	0.47
5:6:612:VAL:HG23	5:6:623:ILE:HA	1.96	0.47
1:2:278:ALA:O	1:2:281:LEU:HG	2.15	0.47
1:2:315:SER:N	1:2:430:TYR:O	2.36	0.47
1:2:785:LYS:HG3	1:2:788:ARG:NH2	2.29	0.47
2:3:342:LEU:O	2:3:346:ASP:HB2	2.14	0.47
4:5:438:TYR:OH	4:5:480:ASP:OD2	2.20	0.47
4:5:626:PHE:HZ	4:5:630:ARG:HH21	1.63	0.47
5:6:124:VAL:HB	5:6:133:GLU:HA	1.95	0.47
5:6:373:MET:HG3	5:6:374:PRO:HD2	1.95	0.47
5:6:609:THR:HG22	5:6:610:ALA:N	2.25	0.47
2:3:201:HIS:CE1	2:3:243:THR:HG22	2.49	0.47
2:3:443:THR:OG1	2:3:457:LEU:HD22	2.15	0.47
3:4:578:LEU:HD22	3:4:630:CYS:HB3	1.96	0.47
3:4:818:GLU:HG3	3:4:820:GLU:H	1.80	0.47
5:6:121:ASP:OD2	5:6:161:ARG:NH2	2.47	0.47
5:6:144:LYS:HZ1	5:6:194:PRO:CG	2.27	0.47
5:6:559:THR:HG23	5:6:565:LEU:HD23	1.95	0.47
5:6:811:ALA:HB2	5:6:819:ILE:HG12	1.96	0.47
6:7:138:VAL:C	6:7:140:ASP:H	2.18	0.47
6:7:628:LEU:N	6:7:629:ASP:HA	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:201:PRO:HG2	1:2:203:VAL:HG23	1.96	0.47
2:3:236:THR:HA	2:3:237:GLU:C	2.33	0.47
3:4:191:THR:OG1	3:4:275:THR:HG22	2.15	0.47
3:4:809:ALA:HB2	3:4:817:VAL:HG23	1.94	0.47
5:6:112:ARG:HH22	5:6:183:LYS:CB	2.27	0.47
5:6:794:ARG:HB2	5:6:795:ILE:C	2.35	0.47
1:2:805:ILE:HD11	1:2:845:PHE:CZ	2.50	0.47
1:2:861:PHE:O	1:2:864:TYR:HB3	2.15	0.47
2:3:176:LEU:HD23	2:3:177:ASN:N	2.30	0.47
3:4:651:GLN:NE2	5:6:586:LYS:NZ	2.62	0.47
3:4:656:ILE:HG23	3:4:658:LYS:HG2	1.97	0.47
3:4:823:GLN:OE1	3:4:823:GLN:N	2.44	0.47
3:4:367:GLU:OE2	5:6:421:LEU:HB3	2.15	0.47
5:6:568:ASP:OD1	5:6:677:SER:HB3	2.14	0.47
5:6:579:THR:HG23	5:6:717:ASP:OD2	2.15	0.47
5:6:768:GLU:OE1	5:6:768:GLU:N	2.47	0.47
3:4:184:ASN:ND2	6:7:141:VAL:HG11	2.30	0.47
6:7:414:LEU:O	6:7:418:ILE:HD12	2.15	0.47
1:2:769:TYR:CZ	1:2:773:LYS:HD3	2.50	0.47
2:3:444:ALA:O	2:3:499:LYS:NZ	2.37	0.47
2:3:670:GLN:HE22	2:3:719:LYS:NZ	2.12	0.47
3:4:249:LEU:HA	3:4:250:ALA:HA	1.60	0.47
3:4:265:PRO:HB3	3:4:325:LEU:HG	1.97	0.47
3:4:455:SER:HB3	6:7:276:ARG:O	2.14	0.47
5:6:767:LYS:HG2	5:6:769:ALA:H	1.79	0.47
6:7:88:TYR:CZ	6:7:92:LYS:HG3	2.49	0.47
1:2:309:LEU:C	1:2:310:ARG:HH11	2.11	0.47
1:2:569:GLN:CD	1:2:613:ASN:HD22	2.18	0.47
1:2:549:LYS:NZ	1:2:651:ASN:OD1	2.47	0.47
1:2:816:ILE:O	1:2:819:SER:OG	2.16	0.47
3:4:557:ARG:NH1	3:4:668:ARG:HH21	2.10	0.47
5:6:819:ILE:HG22	5:6:820:THR:N	2.27	0.47
6:7:484:THR:HG23	6:7:487:GLY:CA	2.44	0.47
2:3:484:VAL:HG22	6:7:528:LYS:HG2	1.97	0.47
2:3:655:PHE:HA	2:3:658:LYS:HZ3	1.80	0.47
3:4:263:ASN:HD21	6:7:135:LYS:HD3	1.80	0.47
3:4:342:MET:HE3	5:6:448:LEU:HD13	1.97	0.47
3:4:796:ARG:HH11	7:6:2001:ADP:H4'	1.79	0.47
4:5:455:ARG:HH12	4:5:460:ARG:HD2	1.78	0.47
6:7:670:ASP:HA	6:7:673:ARG:HG2	1.97	0.47
1:2:338:LYS:HZ3	1:2:376:ASN:HD21	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:152:PRO:HB2	2:3:154:LYS:HE3	1.95	0.47
3:4:334:ARG:NH1	3:4:398:LYS:HD2	2.30	0.47
4:5:239:ASP:HA	4:5:240:PRO:HD2	1.82	0.47
4:5:294:ILE:HG21	4:5:330:ILE:HG12	1.97	0.47
4:5:412:VAL:HB	4:5:520:LEU:HG	1.96	0.47
6:7:451:ARG:HA	6:7:452:GLY:HA3	1.62	0.47
6:7:570:LEU:HB2	6:7:585:ASN:ND2	2.30	0.47
1:2:342:LEU:N	1:2:371:GLY:O	2.47	0.46
1:2:660:THR:O	1:2:850:LYS:HG3	2.15	0.46
2:3:422:VAL:HG11	2:3:513:ILE:HD12	1.96	0.46
3:4:281:VAL:HG22	3:4:297:GLU:HG2	1.97	0.46
3:4:312:LYS:HZ2	3:4:405:PHE:HD2	1.61	0.46
3:4:435:VAL:HG22	3:4:466:VAL:HG22	1.98	0.46
3:4:570:PRO:O	3:4:571:SER:OG	2.29	0.46
3:4:688:VAL:HG12	3:4:692:ILE:HD11	1.96	0.46
4:5:673:GLN:OE1	4:5:675:ARG:NH2	2.47	0.46
5:6:282:GLU:N	5:6:282:GLU:OE1	2.48	0.46
5:6:710:ASP:HA	5:6:711:LEU:HA	1.60	0.46
5:6:777:TYR:CD1	5:6:800:LEU:HB2	2.50	0.46
6:7:257:VAL:HG22	6:7:306:LYS:HB3	1.98	0.46
6:7:83:ASP:OD1	6:7:207:LEU:HB3	2.16	0.46
1:2:435:ASP:N	1:2:436:GLY:HA3	2.30	0.46
3:4:530:ILE:HA	7:4:2001:ADP:C2	2.50	0.46
5:6:426:ILE:HG22	5:6:427:SER:N	2.26	0.46
5:6:769:ALA:O	5:6:772:TYR:HB3	2.16	0.46
1:2:656:ARG:NH1	5:6:794:ARG:HD3	2.29	0.46
2:3:247:TYR:OH	6:7:12:VAL:HG21	2.16	0.46
2:3:347:ILE:HG12	2:3:351:ASN:HD21	1.79	0.46
2:3:524:ASP:O	2:3:532:ASN:ND2	2.47	0.46
3:4:308:VAL:HG21	3:4:325:LEU:HB3	1.97	0.46
4:5:568:ILE:HD11	7:5:2001:ADP:C6	2.51	0.46
4:5:549:ARG:HG2	4:5:651:ARG:NH2	2.31	0.46
5:6:776:LYS:HZ3	5:6:824:ILE:C	2.18	0.46
6:7:25:LEU:HD11	6:7:117:PHE:CE1	2.50	0.46
6:7:158:THR:HB	6:7:185:VAL:HG21	1.97	0.46
1:2:674:LEU:HD21	1:2:680:LEU:HD21	1.97	0.46
2:3:488:GLU:OE2	2:3:492:GLN:HG2	2.16	0.46
4:5:50:LEU:HD22	4:5:101:ILE:HD12	1.97	0.46
4:5:184:ARG:NH1	4:5:240:PRO:HA	2.30	0.46
4:5:535:SER:OG	4:5:538:ASP:OD2	2.21	0.46
5:6:182:GLN:O	5:6:186:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:428:ARG:HD3	5:6:370:THR:O	2.15	0.46
5:6:533:ILE:HD13	5:6:548:LEU:HD13	1.98	0.46
1:2:543:GLY:HA3	1:2:549:LYS:CD	2.37	0.46
2:3:33:ASP:CA	2:3:39:ARG:HH11	2.29	0.46
2:3:467:ARG:NH2	2:3:509:ARG:NH1	2.64	0.46
3:4:318:ASN:ND2	6:7:341:ARG:HH12	2.13	0.46
3:4:404:ASP:OD1	3:4:405:PHE:N	2.49	0.46
3:4:688:VAL:O	3:4:692:ILE:HD12	2.16	0.46
3:4:743:PRO:HG2	3:4:747:LEU:HD23	1.96	0.46
2:3:569:HIS:CD2	4:5:657:ILE:HD13	2.50	0.46
6:7:154:LEU:O	6:7:158:THR:HG22	2.16	0.46
2:3:31:PHE:CD1	2:3:32:LEU:HA	2.50	0.46
4:5:286:VAL:HG13	4:5:290:THR:OG1	2.16	0.46
5:6:162:GLU:O	5:6:163:ASN:HB2	2.15	0.46
1:2:509:ARG:O	1:2:513:THR:OG1	2.21	0.46
1:2:583:ASP:OD2	1:2:590:THR:HG23	2.16	0.46
2:3:437:SER:CB	2:3:438:SER:HA	2.40	0.46
3:4:377:ASN:CB	3:4:378:GLU:HA	2.46	0.46
4:5:486:ARG:O	4:5:490:ARG:HB2	2.16	0.46
6:7:245:ILE:HG12	6:7:315:ILE:HD11	1.98	0.46
6:7:322:VAL:HG21	6:7:328:PRO:HG3	1.97	0.46
1:2:314:LEU:O	1:2:315:SER:OG	2.28	0.46
2:3:555:GLU:O	2:3:558:ASP:HB3	2.15	0.46
3:4:206:ARG:HA	3:4:209:LEU:HB3	1.97	0.46
3:4:462:ASP:OD1	3:4:462:ASP:O	2.33	0.46
4:5:588:GLU:HB3	4:5:593:GLU:HB2	1.97	0.46
5:6:109:GLU:OE2	5:6:112:ARG:HD3	2.15	0.46
5:6:303:GLU:O	5:6:353:PHE:HA	2.16	0.46
5:6:378:ASP:C	5:6:378:ASP:OD1	2.54	0.46
5:6:422:ASP:OD1	5:6:424:ARG:HG3	2.15	0.46
3:4:662:ILE:HD13	5:6:627:ALA:N	2.30	0.46
5:6:603:SER:OG	5:6:644:MET:SD	2.74	0.46
6:7:25:LEU:C	6:7:27:THR:H	2.19	0.46
1:2:305:SER:OG	1:2:306:LEU:N	2.46	0.46
1:2:785:LYS:HG3	1:2:788:ARG:HH21	1.80	0.46
2:3:653:ILE:N	2:3:654:PRO:CD	2.61	0.46
2:3:700:ARG:O	2:3:704:THR:HG23	2.15	0.46
3:4:333:LEU:HD12	3:4:398:LYS:NZ	2.27	0.46
3:4:509:ILE:HG13	3:4:746:PHE:CZ	2.51	0.46
5:6:304:LEU:C	5:6:306:LYS:H	2.18	0.46
6:7:356:LEU:HA	6:7:357:PRO:HD3	1.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:235:ASP:HB2	2:3:241:LEU:HD11	1.98	0.46
3:4:234:ARG:HG3	3:4:291:TYR:OH	2.16	0.46
4:5:27:ILE:O	4:5:30:SER:OG	2.20	0.46
4:5:633:LEU:HB2	4:5:648:ILE:HD11	1.98	0.46
5:6:420:THR:HG22	5:6:445:VAL:HG12	1.98	0.46
5:6:399:GLY:HA2	5:6:454:PHE:CE1	2.50	0.46
5:6:644:MET:HB3	5:6:648:ASP:OD2	2.16	0.46
6:7:28:PHE:CG	6:7:29:LYS:N	2.84	0.46
1:2:271:PHE:HE2	1:2:295:VAL:HG11	1.81	0.45
2:3:330:HIS:HB2	2:3:337:ALA:HB3	1.97	0.45
4:5:549:ARG:HG2	4:5:651:ARG:HH22	1.80	0.45
5:6:130:GLY:HA3	5:6:131:GLU:C	2.36	0.45
5:6:730:HIS:O	5:6:733:ASP:HB2	2.16	0.45
1:2:589:TRP:CH2	4:5:457:PRO:HG3	2.50	0.45
1:2:703:HIS:CD2	5:6:565:LEU:HD22	2.51	0.45
2:3:57:ASN:O	2:3:61:ASP:HB2	2.16	0.45
3:4:471:ASP:HB3	3:4:474:LEU:HG	1.97	0.45
4:5:349:PHE:HZ	4:5:609:LYS:NZ	2.13	0.45
4:5:413:LEU:HD23	4:5:415:LEU:HD23	1.98	0.45
4:5:605:TYR:HE2	4:5:668:LEU:HD11	1.81	0.45
1:2:601:LYS:HZ2	1:2:643:ARG:HD2	1.81	0.45
1:2:794:ARG:O	1:2:797:SER:OG	2.30	0.45
2:3:220:THR:HG21	2:3:224:ARG:HH12	1.82	0.45
3:4:324:LYS:HZ1	6:7:138:VAL:CG1	2.30	0.45
3:4:758:ILE:HD13	3:4:813:LEU:HA	1.98	0.45
5:6:355:ASP:OD2	5:6:383:GLY:CA	2.62	0.45
5:6:537:VAL:HG11	5:6:584:PHE:CE1	2.51	0.45
1:2:576:LEU:HD23	1:2:595:ALA:HB3	1.97	0.45
2:3:409:GLY:H	2:3:415:LYS:HZ3	1.64	0.45
4:5:261:ILE:HG22	4:5:263:GLU:H	1.81	0.45
5:6:356:TRP:HB2	5:6:381:LEU:O	2.17	0.45
6:7:149:ARG:CZ	6:7:152:ARG:HH11	2.25	0.45
6:7:399:GLU:OE2	6:7:403:GLU:OE2	2.35	0.45
6:7:685:THR:HB	6:7:686:PRO:HD2	1.97	0.45
2:3:656:LEU:O	2:3:660:VAL:HG23	2.16	0.45
2:3:673:GLN:HA	2:3:676:ILE:HD12	1.98	0.45
3:4:419:VAL:O	3:4:420:TYR:CD2	2.70	0.45
3:4:641:THR:O	3:4:642:ARG:HB2	2.16	0.45
3:4:712:VAL:HG22	6:7:672:LYS:HZ2	1.80	0.45
4:5:152:ASP:H	4:5:155:HIS:CD2	2.35	0.45
4:5:179:LEU:HD12	4:5:179:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:134:LYS:HG2	5:6:137:ARG:HD3	1.99	0.45
1:2:401:ARG:N	5:6:390:LYS:NZ	2.64	0.45
6:7:209:GLN:HB3	6:7:210:ASN:H	1.63	0.45
6:7:258:ILE:O	6:7:270:PHE:HA	2.15	0.45
6:7:480:GLY:HA2	6:7:520:ILE:O	2.16	0.45
1:2:537:ILE:HG23	1:2:678:ASP:OD2	2.17	0.45
2:3:345:PHE:HE1	2:3:348:ARG:HH21	1.64	0.45
3:4:731:ASP:OD1	3:4:732:LYS:N	2.44	0.45
4:5:363:ASN:HB2	4:5:366:LEU:HB2	1.99	0.45
4:5:66:GLU:HA	4:5:69:ILE:HG22	1.98	0.45
5:6:173:GLN:O	5:6:176:ARG:HB3	2.17	0.45
5:6:288:LEU:N	5:6:399:GLY:HA3	2.28	0.45
5:6:566:ARG:HA	5:6:567:GLY:HA3	1.72	0.45
6:7:213:ARG:O	6:7:215:TYR:CD1	2.69	0.45
6:7:659:TYR:OH	6:7:714:GLU:OE1	2.27	0.45
1:2:397:VAL:HG12	1:2:398:PRO:O	2.17	0.45
1:2:767:ILE:HG13	1:2:768:HIS:H	1.81	0.45
3:4:209:LEU:O	3:4:210:ASP:HB2	2.17	0.45
3:4:211:GLU:HG3	3:4:212:ARG:HG2	1.99	0.45
3:4:267:GLU:O	3:4:271:ILE:HD12	2.15	0.45
4:5:426:LEU:HA	4:5:426:LEU:HD23	1.59	0.45
4:5:356:GLU:CD	4:5:598:LYS:HZ2	2.20	0.45
6:7:19:ASN:O	6:7:22:THR:OG1	2.27	0.45
6:7:466:LYS:HG2	7:7:2001:ADP:O2B	2.17	0.45
6:7:466:LYS:N	7:7:2001:ADP:O2B	2.50	0.45
6:7:516:ALA:O	6:7:561:THR:HG22	2.16	0.45
6:7:668:ARG:HH22	6:7:686:PRO:HD3	1.81	0.45
6:7:581:LEU:HB2	6:7:681:PHE:CE1	2.52	0.45
1:2:811:GLU:CD	1:2:815:ARG:NH1	2.70	0.45
2:3:176:LEU:HA	2:3:298:PHE:HD2	1.82	0.45
2:3:40:ASP:O	2:3:43:ARG:HB3	2.17	0.45
3:4:271:ILE:O	3:4:275:THR:HG23	2.17	0.45
5:6:134:LYS:NZ	5:6:137:ARG:HD2	2.32	0.45
5:6:532:SER:HB3	5:6:745:PRO:HG2	1.99	0.45
5:6:560:VAL:HB	5:6:561:GLU:HA	1.99	0.45
5:6:802:SER:O	5:6:805:ARG:HG2	2.16	0.45
6:7:220:ILE:HA	6:7:223:LYS:HZ2	1.78	0.45
6:7:606:ARG:O	6:7:610:GLU:HG2	2.17	0.45
3:4:337:PRO:HB3	5:6:375:ARG:HD3	1.98	0.45
3:4:662:ILE:HD13	5:6:627:ALA:H	1.82	0.45
4:5:343:TRP:CG	4:5:344:ASN:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:138:VAL:HG22	6:7:139:LEU:N	2.32	0.45
6:7:440:VAL:O	6:7:440:VAL:HG12	2.17	0.45
6:7:709:ASP:O	6:7:712:ASP:HB3	2.16	0.45
1:2:245:ASN:HA	1:2:298:SER:HB2	1.98	0.45
4:5:65:MET:HG2	4:5:76:TYR:CE1	2.52	0.45
5:6:154:ASP:OD1	5:6:155:TYR:N	2.49	0.45
5:6:313:MET:HA	5:6:314:CYS:HA	1.47	0.45
5:6:638:ILE:HG21	5:6:644:MET:HE2	1.98	0.45
1:2:343:LYS:NZ	1:2:371:GLY:N	2.66	0.44
1:2:520:PHE:HD1	1:2:767:ILE:HG22	1.83	0.44
3:4:284:ILE:HA	3:4:290:ASP:OD2	2.17	0.44
3:4:343:LYS:NZ	3:4:392:ALA:HB3	2.32	0.44
3:4:416:SER:O	3:4:460:TYR:HB2	2.17	0.44
5:6:390:LYS:HD2	5:6:391:PRO:HD2	1.97	0.44
3:4:799:GLU:OE1	5:6:735:HIS:NE2	2.50	0.44
5:6:732:VAL:O	5:6:736:MET:HG2	2.16	0.44
6:7:235:LEU:HD12	6:7:355:PHE:CE2	2.52	0.44
6:7:444:VAL:CG2	6:7:448:MET:H	2.29	0.44
1:2:839:LYS:HD2	1:2:839:LYS:HA	1.80	0.44
2:3:245:TYR:C	2:3:247:TYR:H	2.20	0.44
2:3:488:GLU:O	2:3:492:GLN:HB3	2.17	0.44
2:3:730:ALA:O	2:3:734:ARG:HG2	2.17	0.44
3:4:329:LYS:HA	3:4:433:ILE:O	2.17	0.44
3:4:417:LEU:HD22	3:4:463:VAL:HG11	1.99	0.44
3:4:519:TYR:CZ	3:4:538:LYS:HD3	2.51	0.44
4:5:34:PHE:CE1	4:5:68:LEU:HD23	2.52	0.44
5:6:537:VAL:HG11	5:6:584:PHE:CZ	2.51	0.44
1:2:437:ASN:HA	1:2:438:LEU:C	2.37	0.44
3:4:696:PRO:N	3:4:697:PRO:HD2	2.31	0.44
4:5:31:PHE:HE1	4:5:75:ILE:HG21	1.83	0.44
5:6:537:VAL:HA	7:6:2001:ADP:N1	2.33	0.44
1:2:299:ASP:OD1	1:2:301:PRO:HD3	2.17	0.44
2:3:345:PHE:O	2:3:349:ASN:ND2	2.51	0.44
3:4:315:ARG:NH1	6:7:250:ASP:HA	2.33	0.44
3:4:770:LEU:HD21	3:4:802:ILE:HG22	2.00	0.44
4:5:663:LEU:HA	4:5:666:LEU:HD12	1.99	0.44
5:6:625:ALA:CB	5:6:626:GLY:HA2	2.46	0.44
5:6:689:TYR:HA	5:6:690:ASN:CB	2.41	0.44
6:7:2:SER:C	6:7:4:ALA:H	2.21	0.44
1:2:338:LYS:HZ1	1:2:376:ASN:HD21	1.63	0.44
1:2:493:ILE:HG13	1:2:494:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:505:ILE:CD1	1:2:552:ILE:HG13	2.48	0.44
3:4:693:ASP:CG	3:4:694:LEU:H	2.19	0.44
4:5:239:ASP:OD1	4:5:239:ASP:N	2.50	0.44
4:5:387:ALA:HA	4:5:390:CYS:SG	2.58	0.44
6:7:258:ILE:HD12	6:7:271:GLN:HE21	1.83	0.44
6:7:495:ALA:HA	6:7:510:GLY:HA2	1.99	0.44
1:2:325:THR:HG22	1:2:326:ARG:N	2.28	0.44
3:4:428:ARG:HH12	3:4:482:GLU:CG	2.19	0.44
3:4:422:GLU:HG3	3:4:492:HIS:HE1	1.82	0.44
4:5:343:TRP:O	4:5:344:ASN:HB2	2.18	0.44
5:6:749:GLU:HA	5:6:752:ARG:NH2	2.32	0.44
6:7:544:GLN:NE2	6:7:560:ARG:HG2	2.32	0.44
1:2:401:ARG:N	5:6:390:LYS:HZ2	2.16	0.44
1:2:855:ARG:HG3	1:2:858:ARG:NH2	2.32	0.44
2:3:152:PRO:CB	2:3:154:LYS:HE3	2.48	0.44
3:4:235:GLU:HG3	3:4:291:TYR:OH	2.17	0.44
3:4:562:ILE:HB	3:4:703:ASP:OD2	2.18	0.44
5:6:577:PRO:O	5:6:578:SER:HB2	2.18	0.44
6:7:432:LEU:HD13	6:7:473:ILE:HD11	1.99	0.44
6:7:718:ARG:O	6:7:722:VAL:HG23	2.17	0.44
4:5:620:GLU:O	4:5:623:SER:OG	2.22	0.44
4:5:664:ALA:N	4:5:676:HIS:HE1	2.15	0.44
5:6:568:ASP:CG	5:6:569:ILE:H	2.21	0.44
6:7:538:HIS:HD2	6:7:593:ARG:NE	2.16	0.44
2:3:381:ILE:HD11	2:3:418:LEU:HD21	1.99	0.44
3:4:178:ARG:O	3:4:179:ILE:HB	2.16	0.44
3:4:315:ARG:HG2	3:4:410:GLN:HE21	1.81	0.44
3:4:649:MET:HB3	3:4:701:ARG:HD3	1.99	0.44
3:4:799:GLU:O	3:4:802:ILE:HG12	2.18	0.44
4:5:152:ASP:N	4:5:155:HIS:HD2	2.16	0.44
5:6:397:PHE:HE1	5:6:459:VAL:HG13	1.82	0.44
2:3:138:ASP:N	2:3:138:ASP:OD1	2.51	0.43
2:3:672:THR:O	2:3:676:ILE:HD12	2.17	0.43
3:4:532:GLU:HG2	3:4:533:LEU:N	2.32	0.43
4:5:15:GLN:HA	4:5:16:GLY:HA3	1.61	0.43
4:5:421:ALA:HB2	7:5:2001:ADP:C8	2.53	0.43
5:6:420:THR:HG22	5:6:445:VAL:CG1	2.48	0.43
6:7:354:ILE:O	6:7:377:GLU:HB3	2.17	0.43
6:7:393:LEU:HB2	6:7:395:SER:N	2.33	0.43
6:7:470:LEU:CD2	6:7:564:LEU:HD22	2.46	0.43
3:4:573:SER:HA	7:4:2001:ADP:H5'1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:203:TYR:HE1	3:4:222:GLU:HA	1.83	0.43
3:4:318:ASN:ND2	6:7:341:ARG:NH1	2.66	0.43
3:4:463:VAL:O	3:4:463:VAL:HG23	2.17	0.43
4:5:546:ILE:HD12	4:5:546:ILE:H	1.84	0.43
4:5:584:GLN:O	4:5:588:GLU:HG2	2.18	0.43
6:7:131:GLU:N	6:7:131:GLU:OE1	2.50	0.43
6:7:595:ASP:OD1	6:7:595:ASP:N	2.51	0.43
6:7:421:GLU:CA	6:7:625:GLN:HE22	2.31	0.43
1:2:484:PHE:CZ	1:2:766:TYR:HD1	2.36	0.43
2:3:428:LEU:HB3	2:3:429:ALA:HB2	2.00	0.43
2:3:683:TYR:OH	2:3:687:ARG:HD2	2.18	0.43
3:4:346:PHE:CD2	3:4:388:ARG:HB2	2.54	0.43
4:5:198:ASN:OD1	4:5:201:THR:N	2.51	0.43
4:5:635:ILE:HA	4:5:638:LEU:HG	2.00	0.43
5:6:119:LEU:HD11	5:6:188:VAL:HG21	1.99	0.43
5:6:304:LEU:HG	5:6:353:PHE:HE1	1.83	0.43
3:4:473:ARG:NH2	6:7:446:ASP:O	2.51	0.43
2:3:530:HIS:C	2:3:532:ASN:H	2.22	0.43
4:5:149:ARG:HD3	4:5:260:GLU:OE1	2.19	0.43
6:7:208:SER:HB3	6:7:209:GLN:CA	2.49	0.43
1:2:484:PHE:CZ	1:2:766:TYR:CD1	3.06	0.43
1:2:566:ALA:HB1	1:2:576:LEU:HG	2.00	0.43
2:3:389:VAL:CG1	2:3:390:GLU:H	2.13	0.43
3:4:354:HIS:CD2	3:4:372:GLU:HG3	2.46	0.43
5:6:579:THR:N	7:6:2001:ADP:O1A	2.51	0.43
5:6:279:ILE:HD11	5:6:290:ILE:HG12	2.01	0.43
3:4:721:ALA:HB3	6:7:661:VAL:HG13	2.00	0.43
1:2:227:TYR:OH	1:2:248:HIS:ND1	2.34	0.43
1:2:343:LYS:HZ1	1:2:370:LYS:C	2.21	0.43
1:2:481:GLU:O	1:2:484:PHE:HB3	2.18	0.43
3:4:737:SER:HB2	3:4:742:LEU:HD11	1.99	0.43
4:5:602:TYR:O	4:5:605:TYR:HB3	2.18	0.43
1:2:394:PRO:HB2	5:6:673:ASN:ND2	2.34	0.43
2:3:492:GLN:HE22	6:7:471:LYS:HE3	1.84	0.43
2:3:391:LYS:HE2	6:7:620:HIS:O	2.19	0.43
2:3:377:ILE:O	2:3:380:ALA:HB3	2.19	0.43
2:3:536:PRO:HA	2:3:537:ASP:HA	1.67	0.43
3:4:529:SER:O	3:4:723:HIS:NE2	2.31	0.43
4:5:678:ASP:HB3	4:5:682:ARG:HH12	1.83	0.43
6:7:128:PRO:CD	6:7:129:THR:HA	2.49	0.43
6:7:18:PHE:CE1	6:7:119:ARG:NH1	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:225:LEU:H	6:7:241:VAL:HA	1.84	0.43
6:7:441:ASP:OD1	6:7:441:ASP:C	2.57	0.43
6:7:385:LYS:HG2	6:7:639:ARG:HH12	1.83	0.43
1:2:656:ARG:HH11	5:6:794:ARG:CA	2.15	0.43
2:3:130:THR:HG22	2:3:153:TRP:HB2	2.00	0.43
2:3:172:THR:HB	2:3:173:ALA:HA	2.00	0.43
2:3:696:PRO:HB3	6:7:573:ARG:NH1	2.32	0.43
2:3:687:ARG:NH1	2:3:698:THR:HA	2.34	0.43
3:4:402:THR:HA	3:4:403:PRO:HD2	1.86	0.43
4:5:27:ILE:HG22	4:5:31:PHE:CE2	2.54	0.43
6:7:367:LYS:HE3	6:7:367:LYS:HB2	1.87	0.43
6:7:469:LEU:O	6:7:472:ALA:HB3	2.19	0.43
6:7:564:LEU:HD23	6:7:565:ALA:N	2.34	0.43
2:3:500:ALA:H	2:3:501:GLY:HA3	1.83	0.43
2:3:542:ARG:NH1	2:3:700:ARG:CZ	2.82	0.43
3:4:324:LYS:HZ2	6:7:138:VAL:HG11	1.84	0.43
3:4:370:ARG:HH12	5:6:426:ILE:HG13	1.82	0.43
3:4:489:LYS:HG3	3:4:494:GLU:HG3	2.01	0.43
3:4:531:TYR:CE2	3:4:532:GLU:HB2	2.54	0.43
3:4:682:TYR:HB2	3:4:691:ASN:ND2	2.34	0.43
4:5:408:GLY:HA2	4:5:409:ASP:HA	1.72	0.43
4:5:664:ALA:N	4:5:676:HIS:CE1	2.87	0.43
5:6:288:LEU:O	5:6:399:GLY:N	2.51	0.43
6:7:360:TYR:CD2	6:7:373:GLU:HG3	2.54	0.43
6:7:546:ILE:HD12	6:7:557:LEU:HD11	1.99	0.43
1:2:208:ALA:O	1:2:212:LYS:HG2	2.18	0.43
1:2:857:LEU:O	1:2:860:SER:OG	2.27	0.43
2:3:414:ALA:HB2	7:3:2001:ADP:C8	2.54	0.43
2:3:480:ASP:OD1	2:3:481:VAL:N	2.52	0.43
3:4:769:GLU:O	3:4:772:ARG:HG2	2.19	0.43
3:4:811:MET:O	3:4:812:LYS:HB2	2.18	0.43
4:5:19:PRO:HB2	4:5:20:ASN:C	2.40	0.43
4:5:319:SER:OG	4:5:320:GLY:N	2.52	0.43
4:5:65:MET:O	4:5:68:LEU:HB2	2.19	0.43
4:5:663:LEU:O	4:5:666:LEU:HB2	2.19	0.43
6:7:394:THR:HG22	6:7:394:THR:O	2.18	0.43
1:2:212:LYS:O	1:2:215:LEU:HB3	2.19	0.42
1:2:233:THR:O	1:2:235:GLY:HA3	2.19	0.42
2:3:100:LEU:HB2	2:3:159:GLY:HA2	2.01	0.42
2:3:487:HIS:NE2	2:3:539:LEU:HG	2.34	0.42
2:3:656:LEU:O	2:3:659:TYR:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:698:THR:HG21	6:7:462:PRO:HG2	2.01	0.42
2:3:727:LYS:O	2:3:730:ALA:HB3	2.19	0.42
4:5:62:THR:HA	4:5:138:ILE:O	2.18	0.42
5:6:653:HIS:HB2	5:6:705:ILE:HG22	2.01	0.42
6:7:318:LEU:O	6:7:319:SER:OG	2.25	0.42
6:7:559:ALA:HB1	6:7:561:THR:HG23	2.01	0.42
6:7:671:SER:O	6:7:674:GLU:HB3	2.19	0.42
1:2:856:GLN:NE2	1:2:859:ARG:HD3	2.33	0.42
5:6:550:GLN:HA	5:6:569:ILE:CG2	2.49	0.42
2:3:287:LYS:HB3	6:7:326:HIS:ND1	2.34	0.42
2:3:519:VAL:HG23	2:3:532:ASN:O	2.19	0.42
2:3:703:GLU:HB3	2:3:707:ARG:NH2	2.34	0.42
3:4:419:VAL:O	3:4:420:TYR:CG	2.72	0.42
4:5:614:LEU:HA	4:5:672:ALA:HB3	2.00	0.42
6:7:284:CYS:HB2	6:7:296:GLY:O	2.19	0.42
6:7:465:ALA:HA	7:7:2001:ADP:O2A	2.19	0.42
1:2:839:LYS:HZ2	1:2:864:TYR:HA	1.83	0.42
2:3:467:ARG:CZ	2:3:509:ARG:NH1	2.82	0.42
2:3:558:ASP:OD1	4:5:626:PHE:CD2	2.73	0.42
4:5:264:LEU:HB2	4:5:265:VAL:CG2	2.43	0.42
4:5:374:ILE:HG23	4:5:428:PHE:CE2	2.55	0.42
6:7:459:MET:HG3	6:7:460:GLY:N	2.34	0.42
6:7:385:LYS:HE2	6:7:478:PRO:HA	2.01	0.42
6:7:68:GLN:O	6:7:71:ALA:N	2.53	0.42
2:3:201:HIS:ND1	2:3:243:THR:HG22	2.35	0.42
2:3:530:HIS:O	2:3:531:GLN:HB2	2.19	0.42
3:4:400:GLN:NE2	6:7:555:THR:HG22	2.34	0.42
3:4:567:CYS:HB3	3:4:675:ALA:HB3	2.00	0.42
3:4:794:THR:HG23	3:4:796:ARG:H	1.85	0.42
4:5:379:PHE:N	7:5:2001:ADP:HN62	2.11	0.42
4:5:413:LEU:HA	4:5:521:ALA:O	2.20	0.42
5:6:123:SER:HB2	5:6:135:VAL:N	2.30	0.42
5:6:664:ALA:HB2	5:6:669:HIS:CD2	2.54	0.42
5:6:786:GLN:HA	5:6:787:GLY:HA2	1.80	0.42
1:2:803:PHE:HB2	1:2:804:PRO:HA	2.01	0.42
2:3:372:TYR:CE1	2:3:564:HIS:HB3	2.55	0.42
3:4:728:TYR:CG	3:4:729:LEU:N	2.86	0.42
3:4:774:TYR:HE1	3:4:795:THR:HA	1.85	0.42
5:6:765:LEU:CD2	5:6:770:ARG:HB3	2.49	0.42
5:6:817:ASP:C	5:6:819:ILE:H	2.22	0.42
6:7:499:LYS:NZ	6:7:504:ASP:OD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:664:TYR:CD1	6:7:689:LEU:HB2	2.54	0.42
1:2:210:GLU:O	1:2:213:SER:HB3	2.19	0.42
2:3:97:ILE:HG21	2:3:158:LYS:HE3	2.02	0.42
2:3:259:GLN:HB2	4:5:461:GLU:OE2	2.19	0.42
3:4:419:VAL:HA	3:4:463:VAL:CG2	2.49	0.42
3:4:557:ARG:HE	3:4:668:ARG:HH21	1.67	0.42
5:6:379:VAL:HG11	5:6:397:PHE:HE2	1.85	0.42
1:2:405:HIS:HB2	5:6:621:TYR:CD1	2.54	0.42
6:7:82:LEU:HD12	6:7:206:PRO:HA	2.02	0.42
6:7:627:ASP:OD1	6:7:628:LEU:N	2.53	0.42
6:7:83:ASP:O	6:7:86:LEU:HB3	2.20	0.42
1:2:341:CYS:O	1:2:342:LEU:HD12	2.20	0.42
2:3:43:ARG:HB2	2:3:136:MET:HE2	2.02	0.42
2:3:388:GLY:HA2	2:3:710:THR:HB	2.01	0.42
3:4:571:SER:H	7:4:2001:ADP:PB	2.43	0.42
4:5:194:ILE:O	4:5:194:ILE:HG13	2.20	0.42
4:5:181:ILE:HG21	4:5:241:TYR:HB3	2.02	0.42
4:5:440:SER:OG	4:5:480:ASP:HB2	2.19	0.42
4:5:407:ARG:HD3	4:5:498:GLU:O	2.20	0.42
4:5:652:GLN:O	4:5:655:ALA:HB3	2.19	0.42
4:5:607:ARG:HA	4:5:665:LYS:NZ	2.35	0.42
6:7:349:VAL:HG23	6:7:383:GLN:HA	2.02	0.42
6:7:680:SER:CB	6:7:681:PHE:HA	2.50	0.42
1:2:208:ALA:HB1	1:2:274:VAL:HG21	2.01	0.42
1:2:544:ASP:OD2	1:2:656:ARG:HB2	2.20	0.42
2:3:476:ASP:CA	2:3:483:ARG:HH12	2.29	0.42
3:4:284:ILE:HG23	3:4:290:ASP:OD2	2.20	0.42
3:4:484:GLU:OE1	5:6:275:ARG:NH2	2.53	0.42
3:4:545:PHE:CE1	3:4:751:ILE:HG23	2.55	0.42
3:4:758:ILE:CD1	3:4:813:LEU:HA	2.50	0.42
4:5:663:LEU:HB3	4:5:676:HIS:CE1	2.55	0.42
5:6:177:PHE:O	5:6:181:LEU:HD13	2.20	0.42
5:6:600:GLY:HA2	5:6:601:LYS:C	2.40	0.42
5:6:640:GLU:N	5:6:681:ALA:O	2.47	0.42
5:6:689:TYR:HD2	5:6:716:LEU:HD12	1.85	0.42
5:6:777:TYR:CZ	5:6:781:ARG:HD2	2.55	0.42
1:2:656:ARG:HG3	1:2:657:TYR:N	2.35	0.42
1:2:804:PRO:HD2	1:2:845:PHE:HE1	1.85	0.42
2:3:433:THR:HG22	2:3:473:ASP:HB2	2.02	0.42
3:4:233:MET:SD	3:4:241:LEU:HB2	2.59	0.42
3:4:568:GLY:O	3:4:574:LYS:NZ	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:25:THR:C	4:5:27:ILE:H	2.23	0.42
4:5:577:THR:HA	4:5:579:ASN:N	2.35	0.42
5:6:575:GLY:H	5:6:581:LYS:HZ3	1.67	0.42
6:7:208:SER:CB	6:7:209:GLN:HG3	2.50	0.42
6:7:247:ARG:O	6:7:248:VAL:HG12	2.20	0.42
6:7:481:VAL:CG2	6:7:516:ALA:HB2	2.50	0.42
1:2:621:HIS:CE1	4:5:481:GLU:OE2	2.73	0.41
3:4:179:ILE:HG12	3:4:180:ILE:O	2.20	0.41
3:4:408:ASP:C	3:4:410:GLN:N	2.73	0.41
3:4:604:TYR:HD2	3:4:617:GLU:OE1	2.03	0.41
3:4:679:GLY:HA3	3:4:681:ARG:O	2.20	0.41
3:4:763:THR:O	3:4:767:LYS:NZ	2.53	0.41
4:5:585:ASN:O	4:5:589:GLU:HG2	2.20	0.41
5:6:370:THR:HA	5:6:371:GLY:HA2	1.73	0.41
5:6:358:LYS:HD2	5:6:378:ASP:OD2	2.20	0.41
5:6:759:ARG:CA	5:6:812:ARG:HH21	2.30	0.41
6:7:479:ARG:HG3	6:7:479:ARG:O	2.20	0.41
1:2:201:PRO:HB2	1:2:202:ASN:H	1.63	0.41
1:2:311:GLU:O	1:2:314:LEU:HG	2.21	0.41
1:2:794:ARG:HD3	4:5:565:ASP:OD2	2.20	0.41
2:3:171:LEU:O	2:3:172:THR:OG1	2.33	0.41
2:3:666:ARG:HA	2:3:667:VAL:HA	1.69	0.41
3:4:303:VAL:HG12	3:4:305:PRO:HD3	2.03	0.41
3:4:352:CYS:N	3:4:353:ASP:HA	2.35	0.41
3:4:415:ILE:HG22	3:4:416:SER:N	2.36	0.41
3:4:641:THR:HG22	3:4:642:ARG:H	1.85	0.41
4:5:166:ILE:HD11	4:5:256:LEU:HD23	2.02	0.41
4:5:453:VAL:CG1	4:5:509:ILE:HD11	2.50	0.41
1:2:693:GLU:HG3	5:6:778:LYS:NZ	2.34	0.41
6:7:13:ASP:O	6:7:17:LEU:HD13	2.20	0.41
1:2:534:ARG:HG2	1:2:536:ASP:H	1.85	0.41
1:2:596:LEU:HD13	1:2:623:ALA:HB2	2.02	0.41
1:2:760:GLN:O	1:2:763:LEU:HG	2.19	0.41
2:3:27:ARG:NH1	2:3:106:PHE:CE2	2.88	0.41
2:3:300:SER:HA	2:3:319:THR:HG22	2.01	0.41
3:4:245:ALA:HA	3:4:246:ARG:HA	1.61	0.41
3:4:267:GLU:O	3:4:270:SER:OG	2.20	0.41
3:4:502:THR:HG22	3:4:503:ASP:N	2.35	0.41
3:4:774:TYR:CE1	3:4:795:THR:HA	2.55	0.41
4:5:264:LEU:HA	4:5:265:VAL:HA	1.81	0.41
4:5:677:VAL:HG12	4:5:681:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:606:ALA:HA	5:6:607:GLY:C	2.39	0.41
5:6:642:ASP:OD2	5:6:683:ASN:O	2.37	0.41
5:6:685:VAL:HG23	5:6:698:ASN:O	2.20	0.41
5:6:786:GLN:OE1	5:6:787:GLY:HA2	2.19	0.41
1:2:770:ALA:O	1:2:774:ILE:HG22	2.20	0.41
1:2:843:ASP:C	1:2:843:ASP:OD1	2.59	0.41
2:3:413:THR:HG22	2:3:413:THR:O	2.21	0.41
3:4:260:GLN:O	3:4:268:VAL:HG21	2.20	0.41
3:4:557:ARG:HH11	3:4:668:ARG:CZ	2.30	0.41
4:5:165:ILE:HD12	4:5:262:PRO:HD2	2.01	0.41
4:5:571:HIS:O	4:5:575:ILE:HG13	2.20	0.41
5:6:577:PRO:HA	7:6:2001:ADP:O1B	2.21	0.41
3:4:370:ARG:NH2	5:6:426:ILE:HG13	2.35	0.41
1:2:233:THR:C	1:2:235:GLY:HA3	2.41	0.41
1:2:446:VAL:HG21	5:6:356:TRP:CZ2	2.56	0.41
2:3:447:THR:HA	2:3:448:THR:HA	1.71	0.41
2:3:468:GLY:O	2:3:511:SER:OG	2.27	0.41
3:4:246:ARG:O	3:4:246:ARG:HG3	2.20	0.41
4:5:530:TYR:HD1	4:5:533:LEU:HD12	1.85	0.41
4:5:543:GLN:HG3	4:5:546:ILE:CD1	2.51	0.41
1:2:447:PHE:CE2	5:6:304:LEU:HD11	2.55	0.41
5:6:304:LEU:O	5:6:305:TYR:CD2	2.73	0.41
5:6:569:ILE:HG13	5:6:570:ASN:N	2.36	0.41
6:7:517:ASP:N	6:7:517:ASP:OD1	2.52	0.41
1:2:260:LEU:HD23	1:2:267:MET:HG2	2.02	0.41
1:2:406:ARG:HH11	1:2:430:TYR:HE1	1.68	0.41
3:4:313:GLY:CA	3:4:403:PRO:HB3	2.51	0.41
3:4:572:THR:HG22	3:4:572:THR:O	2.21	0.41
3:4:650:GLU:OE2	3:4:796:ARG:NH1	2.50	0.41
4:5:305:ASN:HB2	4:5:319:SER:HB3	2.01	0.41
4:5:278:CYS:SG	4:5:330:ILE:HD12	2.60	0.41
5:6:426:ILE:CG2	5:6:427:SER:H	2.24	0.41
5:6:537:VAL:HG21	5:6:584:PHE:CE1	2.55	0.41
6:7:242:ARG:HA	6:7:349:VAL:O	2.20	0.41
6:7:318:LEU:O	6:7:318:LEU:HD23	2.21	0.41
6:7:570:LEU:HD13	6:7:585:ASN:ND2	2.34	0.41
1:2:309:LEU:N	1:2:310:ARG:NH1	2.65	0.41
1:2:557:GLU:CD	1:2:565:PHE:HB2	2.40	0.41
1:2:811:GLU:HG2	4:5:576:HIS:NE2	2.35	0.41
2:3:261:MET:HB3	2:3:264:MET:HB3	2.03	0.41
2:3:442:LEU:O	2:3:460:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:230:LEU:HD21	3:4:280:MET:SD	2.60	0.41
3:4:347:PHE:CZ	3:4:384:LEU:HD12	2.56	0.41
3:4:649:MET:CB	3:4:701:ARG:HD3	2.51	0.41
3:4:762:ILE:HG12	5:6:736:MET:CE	2.46	0.41
5:6:143:MET:CE	5:6:148:LEU:HB2	2.51	0.41
5:6:290:ILE:HD13	5:6:454:PHE:CE1	2.56	0.41
5:6:689:TYR:HB3	5:6:691:ARG:N	2.35	0.41
5:6:772:TYR:CE2	5:6:776:LYS:HE3	2.55	0.41
1:2:609:PHE:HB3	1:2:669:LEU:HD21	2.02	0.41
2:3:435:ARG:HA	2:3:436:GLY:HA3	1.65	0.41
2:3:450:ARG:N	2:3:451:GLU:HA	2.36	0.41
2:3:686:LEU:HD21	2:3:734:ARG:NH2	2.36	0.41
3:4:276:ILE:O	3:4:280:MET:HG2	2.21	0.41
3:4:561:ASP:OD1	3:4:670:SER:HA	2.21	0.41
3:4:777:MET:SD	3:4:830:ARG:NE	2.93	0.41
1:2:693:GLU:HA	5:6:778:LYS:HZ1	1.84	0.41
5:6:767:LYS:NZ	5:6:820:THR:HA	2.35	0.41
6:7:523:ILE:HG21	6:7:526:PHE:HD1	1.84	0.41
6:7:529:MET:HE1	6:7:537:ILE:HD12	2.02	0.41
6:7:476:ILE:O	6:7:639:ARG:HD3	2.20	0.41
1:2:440:ALA:O	1:2:442:ASN:ND2	2.53	0.41
1:2:533:ILE:HG22	1:2:534:ARG:H	1.85	0.41
1:2:616:ASP:O	1:2:619:SER:OG	2.15	0.41
3:4:646:HIS:HE1	3:4:698:LEU:HB2	1.85	0.41
3:4:569:ASP:OD1	3:4:681:ARG:HA	2.21	0.41
4:5:414:LEU:HD23	4:5:414:LEU:HA	1.90	0.41
1:2:338:LYS:HZ1	1:2:376:ASN:ND2	2.19	0.41
1:2:429:ILE:O	1:2:429:ILE:HG13	2.19	0.41
1:2:547:THR:HG22	1:2:548:ALA:N	2.36	0.41
1:2:661:LEU:HB3	1:2:662:PRO:HD2	2.02	0.41
2:3:101:ASP:HA	2:3:104:ARG:NH2	2.29	0.41
2:3:440:VAL:HG12	2:3:441:GLY:N	2.36	0.41
3:4:454:LYS:O	3:4:454:LYS:HG2	2.21	0.41
3:4:713:ASP:CB	3:4:716:ASN:HB2	2.44	0.41
5:6:645:ASP:HB3	5:6:646:ILE:H	1.68	0.41
6:7:149:ARG:NH1	6:7:152:ARG:NE	2.65	0.41
1:2:307:ARG:HG3	1:2:308:GLU:HG2	2.03	0.41
2:3:671:LEU:HD22	6:7:621:MET:HB2	2.03	0.41
3:4:497:GLU:HG3	3:4:498:VAL:HG23	2.03	0.41
3:4:636:LYS:HB2	3:4:636:LYS:HE2	1.78	0.41
3:4:832:ALA:HB1	3:4:836:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:266:PRO:C	4:5:268:GLY:H	2.24	0.41
4:5:464:LEU:HD23	4:5:466:GLY:N	2.36	0.41
4:5:3:PHE:HB3	4:5:4:ASP:H	1.45	0.41
2:3:464:LEU:HD23	4:5:510:THR:HG21	2.02	0.41
5:6:326:LYS:H	5:6:327:TYR:HA	1.85	0.41
5:6:363:GLU:OE2	5:6:367:GLU:HB3	2.21	0.41
5:6:373:MET:CG	5:6:374:PRO:HD2	2.50	0.41
1:2:505:ILE:C	1:2:507:GLY:H	2.23	0.40
1:2:544:ASP:H	1:2:549:LYS:HD3	1.85	0.40
2:3:414:ALA:O	2:3:417:GLN:N	2.54	0.40
4:5:473:ASP:OD1	4:5:474:GLY:N	2.54	0.40
4:5:675:ARG:HA	4:5:678:ASP:OD2	2.21	0.40
6:7:465:ALA:CA	7:7:2001:ADP:H5'1	2.50	0.40
6:7:63:TYR:HD1	6:7:66:MET:HE2	1.86	0.40
1:2:528:ASN:HA	1:2:529:GLY:HA2	1.50	0.40
2:3:252:ASP:OD2	6:7:231:LYS:HD2	2.22	0.40
3:4:284:ILE:HG23	3:4:290:ASP:HB2	2.03	0.40
3:4:325:LEU:HA	3:4:325:LEU:HD23	1.94	0.40
3:4:354:HIS:HB3	3:4:372:GLU:HG2	2.03	0.40
4:5:69:ILE:HB	4:5:76:TYR:CG	2.56	0.40
5:6:559:THR:O	5:6:560:VAL:HG22	2.21	0.40
6:7:106:ILE:O	6:7:110:ALA:HB2	2.20	0.40
6:7:214:ARG:CD	6:7:215:TYR:O	2.69	0.40
6:7:654:GLU:O	6:7:657:ASN:HB3	2.21	0.40
1:2:342:LEU:HD11	1:2:374:ARG:NH1	2.36	0.40
2:3:237:GLU:O	2:3:239:ASN:N	2.54	0.40
4:5:337:VAL:HA	4:5:338:GLU:HA	1.74	0.40
5:6:284:ILE:HD11	5:6:403:VAL:CG2	2.51	0.40
5:6:777:TYR:CE1	5:6:781:ARG:HD2	2.57	0.40
6:7:290:SER:C	6:7:292:ASN:H	2.24	0.40
6:7:339:LEU:HD11	6:7:381:VAL:HG23	2.02	0.40
6:7:441:ASP:O	6:7:442:LYS:HB2	2.21	0.40
6:7:452:GLY:H	6:7:694:ARG:HD2	1.86	0.40
3:4:718:ARG:HA	6:7:665:ILE:HD11	2.03	0.40
2:3:330:HIS:CD2	2:3:337:ALA:H	2.39	0.40
2:3:44:SER:O	2:3:47:VAL:HB	2.22	0.40
3:4:366:GLN:O	3:4:366:GLN:HG2	2.21	0.40
3:4:422:GLU:HG3	3:4:492:HIS:CE1	2.56	0.40
3:4:563:ASN:O	3:4:703:ASP:HB3	2.20	0.40
4:5:453:VAL:HG11	4:5:509:ILE:HD11	2.03	0.40
4:5:442:LYS:HD3	4:5:486:ARG:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:752:ARG:C	5:6:756:LYS:NZ	2.74	0.40
5:6:779:GLU:HA	5:6:782:LYS:HZ1	1.86	0.40
6:7:89:GLN:NE2	6:7:101:ASP:HA	2.37	0.40
6:7:238:LEU:HA	6:7:354:ILE:HA	2.04	0.40
6:7:472:ALA:O	6:7:476:ILE:HD12	2.22	0.40
6:7:540:VAL:O	6:7:540:VAL:HG12	2.22	0.40
1:2:777:LYS:H	1:2:828:PHE:HA	1.86	0.40
2:3:421:PHE:CD1	4:5:402:ASP:OD2	2.74	0.40
3:4:258:TYR:CZ	3:4:262:LEU:HD11	2.57	0.40
5:6:153:ILE:HD11	5:6:267:PHE:CE1	2.57	0.40
5:6:153:ILE:O	5:6:267:PHE:HA	2.20	0.40
5:6:574:VAL:HB	5:6:714:VAL:HG22	2.04	0.40
3:4:411:THR:HG21	6:7:508:LEU:O	2.20	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 PDB entries followed by that with respect to all EM entries.

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	2	597/868 (69%)	544 (91%)	47 (8%)	6 (1%)	18	61
2	3	595/971 (61%)	548 (92%)	40 (7%)	7 (1%)	15	58
3	4	632/933 (68%)	554 (88%)	71 (11%)	7 (1%)	17	60
4	5	621/775 (80%)	586 (94%)	32 (5%)	3 (0%)	32	73
5	6	608/1017 (60%)	547 (90%)	52 (9%)	9 (2%)	12	53
6	7	681/845 (81%)	619 (91%)	52 (8%)	10 (2%)	12	53
All	All	3734/5409 (69%)	3398 (91%)	294 (8%)	42 (1%)	21	60

All (42) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
3	4	189	GLU
3	4	609	VAL
4	5	596	ILE
5	6	317	ILE
6	7	26	VAL
6	7	209	GLN
6	7	464	VAL
6	7	544	GLN
1	2	297	ILE
2	3	230	ILE
2	3	389	VAL
3	4	179	ILE
3	4	419	VAL
3	4	494	GLU
4	5	267	VAL
4	5	410	ILE
5	6	321	VAL
5	6	402	ILE
5	6	426	ILE
5	6	541	GLU
5	6	560	VAL
5	6	819	ILE
6	7	371	LEU
6	7	374	THR
1	2	305	SER
2	3	336	VAL
5	6	305	TYR
1	2	291	SER
1	2	533	ILE
1	2	585	ILE
3	4	493	ASN
6	7	375	TYR
6	7	502	VAL
2	3	440	VAL
5	6	569	ILE
6	7	678	LYS
1	2	372	PRO
2	3	238	GLY
3	4	463	VAL
2	3	519	VAL
6	7	248	VAL
2	3	326	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 PDB entries followed by that with respect to all EM entries.

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	2	509/770 (66%)	509 (100%)	0	100	100
2	3	523/835 (63%)	523 (100%)	0	100	100
3	4	573/848 (68%)	572 (100%)	1 (0%)	94	98
4	5	566/688 (82%)	566 (100%)	0	100	100
5	6	497/886 (56%)	497 (100%)	0	100	100
6	7	609/753 (81%)	608 (100%)	1 (0%)	94	98
All	All	3277/4780 (69%)	3275 (100%)	2 (0%)	95	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4	442	ILE
6	7	214	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	313	ASN
1	2	333	GLN
1	2	376	ASN
1	2	437	ASN
1	2	613	ASN
1	2	658	ASN
1	2	809	HIS
1	2	849	GLN
1	2	856	GLN
2	3	175	HIS
2	3	330	HIS
2	3	349	ASN
2	3	351	ASN
2	3	374	HIS
2	3	404	ASN

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Mol	Chain	Res	Type
2	3	492	GLN
2	3	493	GLN
2	3	554	ASN
2	3	569	HIS
2	3	670	GLN
2	3	688	ASN
3	4	247	ASN
3	4	263	ASN
3	4	274	GLN
3	4	318	ASN
3	4	354	HIS
3	4	410	GLN
3	4	465	HIS
3	4	646	HIS
3	4	651	GLN
3	4	757	HIS
3	4	808	HIS
4	5	49	GLN
4	5	140	ASN
4	5	155	HIS
4	5	254	GLN
4	5	411	ASN
4	5	494	HIS
4	5	543	GLN
4	5	585	ASN
4	5	676	HIS
5	6	149	ASN
5	6	690	ASN
5	6	698	ASN
5	6	750	GLN
6	7	87	GLN
6	7	89	GLN
6	7	90	ASN
6	7	124	ASN
6	7	144	ASN
6	7	292	ASN
6	7	334	HIS
6	7	379	GLN
6	7	538	HIS
6	7	544	GLN
6	7	554	ASN
6	7	585	ASN

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Mol	Chain	Res	Type
6	7	620	HIS
6	7	622	HIS

### 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 ⓘ

6 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	$\# Z  > 2$
7	ADP	2	2001	-	25,29,29	0.93	1 (4%)	24,45,45	1.76	2 (8%)
7	ADP	3	2001	-	25,29,29	0.98	1 (4%)	24,45,45	1.63	2 (8%)
7	ADP	4	2001	-	25,29,29	0.94	1 (4%)	24,45,45	1.59	2 (8%)
7	ADP	5	2001	-	25,29,29	0.94	1 (4%)	24,45,45	1.67	2 (8%)
7	ADP	6	2001	-	25,29,29	0.99	1 (4%)	24,45,45	1.76	3 (12%)
7	ADP	7	2001	-	25,29,29	0.96	1 (4%)	24,45,45	1.60	2 (8%)

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
7	ADP	2	2001	-	-	0/12/32/32	0/3/3/3
7	ADP	3	2001	-	-	0/12/32/32	0/3/3/3
7	ADP	4	2001	-	-	0/12/32/32	0/3/3/3
7	ADP	5	2001	-	-	0/12/32/32	0/3/3/3
7	ADP	6	2001	-	-	0/12/32/32	0/3/3/3
7	ADP	7	2001	-	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	5	2001	ADP	C5-C4	2.82	1.46	1.40
7	4	2001	ADP	C5-C4	2.84	1.46	1.40
7	7	2001	ADP	C5-C4	2.88	1.47	1.40
7	2	2001	ADP	C5-C4	2.91	1.47	1.40
7	3	2001	ADP	C5-C4	2.92	1.47	1.40
7	6	2001	ADP	C5-C4	3.23	1.47	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	2	2001	ADP	N3-C2-N1	-6.61	123.10	128.86
7	6	2001	ADP	N3-C2-N1	-6.13	123.52	128.86
7	3	2001	ADP	N3-C2-N1	-5.71	123.88	128.86
7	5	2001	ADP	N3-C2-N1	-5.69	123.91	128.86
7	7	2001	ADP	N3-C2-N1	-5.67	123.92	128.86
7	4	2001	ADP	N3-C2-N1	-5.37	124.18	128.86
7	4	2001	ADP	C4-C5-N7	-3.08	106.43	109.41
7	6	2001	ADP	C4-C5-N7	-2.69	106.81	109.41
7	5	2001	ADP	C4-C5-N7	-2.65	106.84	109.41
7	7	2001	ADP	C4-C5-N7	-2.59	106.91	109.41
7	3	2001	ADP	C4-C5-N7	-2.53	106.96	109.41
7	2	2001	ADP	C4-C5-N7	-2.46	107.04	109.41
7	6	2001	ADP	C4'-O4'-C1'	2.32	112.24	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	2	2001	ADP	1	0
7	3	2001	ADP	4	0
7	4	2001	ADP	6	0
7	5	2001	ADP	7	0
7	6	2001	ADP	10	0
7	7	2001	ADP	6	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.